APPLICATION

For

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on

CRYSTAL STRUCTURES OF *T. FOETUS* INOSINE MONOPHOSPHATE DEHYDROGENASE IN COMPLEX WITH SUBSTRATE, COFACTOR AND ANALOGS AND USES THEREOF

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CRYSTAL STRUCTURES OF T. FOETUS INOSINE MONOPHOSPHATE DEHYDROGENASE IN COMPLEX WITH SUBSTRATE, COFACTOR AND ANALOGS AND USES THEREOF

This application claims benefit of the filing date of U.S. Provisional Application No. 60/410,523, filed September 13, 2002, and U.S. Provisional Application No. 60/412,044, filed September 18, 2002, both of which are incorporated herein by reference.

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BACKGROUND OF THE INVENTION

This invention relates generally to drug development and, more specifically, to designing compounds that modulate inosine monophosphate dehydrogenase.

The enzyme inosine monophosphate dehydrogenase (IMPDH) is responsible for the rate-limiting step in guanine nucleotide biosynthesis. Because it is upregulated in rapidly proliferating cells, human type II IMPDH is actively targeted for immunosuppressive, anticancer, and antiviral chemotherapy. The enzyme employs a random-in ordered-out kinetic mechanism where substrate or cofactor can bind first but product is only released after the cofactor leaves. Due to structural and kinetic differences between mammalian and microbial enzymes, most drugs that are successful in the inhibition of mammalian IMPDH are far less effective against the microbial forms of the enzyme. However, with greater knowledge of the structural mechanism of the microbial

enzymes, more effective and selective inhibitors of microbial IMPDH can be developed for use as anti-microbial drugs.

Thus, there exists a need for identifying and designing compounds that modulate IMPDH activity. The present invention satisfies this need and provides related advantages as well.

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SUMMARY OF THE INVENTION

The invention provides a crystalline complex containing T. foetus inosine monophospate dehydrogenase (IMPDH) in complex with inosine monophosphate (IMP), the complex specified by disclosed atomic coordinates. Also provided are crystalline complexes of containing T. foetus IMPDH with both inosine monophosphate (IMP) and mycophenolic acid, with both xanthosine monophosphate (XMP) and mycophenolic acid, with both xanthosine monophosphate (XMP) and nicotinic adenine dinucleotide (NAD), with ribovirin $(1-\beta-D-ribofuranosyl-1,2,4$ triazole-3-carboxamide), and with both ribovirin and mycophenolic acid, each complex specified by disclosed atomic coordinates. The T. foetus IMPDH structures have complete active sites. Also provided by the invention are the atomic coordinates for these complexes. Further provided by the invention are methods for identifying a modulator of IMPDH that employ the atomic coordinates of the invention.

The invention provides methods for identifying an inhibitor of IMPDH. In one embodiment, a method of the invention involves displaying a structure for IMPDH, or a portion thereof, wherein the structure has a set of atomic coordinates shown in Tables 2-7; (b) docking a structure of a candidate inhibitor to the structure of IMPDH, or the portion thereof; and (c) identifying an inhibitor of IMPDH, wherein the inhibitor has a structure that docks favorably to the structure of IMPDH, or the portion thereof. In one embodiment, the method is used to identify an inhibitor that targets the substrate binding site to which IMP or XMP binds. In another embodiment, the method is used to identify an inhibitor that targets the NAD cofactor binding site to which NAD or MOA binds. In a further embodiment, the method can include docking a candidate inhibitor to a second IMPDH structure.

In another embodiment, the invention provides a

method of identifying an inhibitor of IMPDH that involves
displaying the structure for the bound complex of T.

foetus IMPDH with NAD set forth in Table 5, (b) docking a
structure of a candidate inhibitor to said structure, or
portion thereof; and identifying a compound that binds

Asp-358 and Asp-261, wherein said compound has a
structure that docks favorably to said structure, or
portion thereof.

In a further embodiment, the invention provides a

method of identifying an inhibitor of IMPDH that involves

(a) selecting a candidate compound by performing rational
drug design with a set of atomic coordinates set forth in

Tables 2-7, wherein said selecting is performed in conjunction with computer modeling; (b) contacting said compound with IMPDH, and (c) determining the ability of said compound to reduce IMPDH activity, wherein a compound that reduces IMPDH activity is an inhibitor of IMPDH.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 shows IMPDH crystals from the original ammonium sulfate condition (left) compared with those grown from the sodium malonate (right). In malonate, the crystals grew to 0.4-0.8 mm in length while the sulfate crystals grew to between 0.1 and 0.4 mm. The sulfate-grown crystals were also much more fragile. Further, the malonate in the mother liquor acted as a cryoprotectant. No detectable needle-shaped crystals, which were observed in the sulfate condition, were observed in the malonate condition.

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Figure 2 shows a ribbon diagram of the IMPDH tetramer viewed along the four-fold axis. The enzyme is in complex with the product XMP (light shading), the cofactor NAD⁺ (dark shading) and the potassium. Although the cofactor lies along the dimer interface, it does not make contact with the neighboring monomer. All molecular images were prepared with the program Deepview and rendered in POVRAY 3.5 beta.

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Figure 3 shows the active site loop of T. foetus IMPDH. A 2.2 Å resolution $2F_o-F_c$ electron density map contoured at 0.5 σ surrounds a model of the active

site loop from the IMP-bound structure. The low contouring level is necessary to obtain continuous electron density.

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Figure 4 shows that a potassium ion was located at the dimer interface near the cofactor binding site. The carbon atoms of the neighboring monomer are shaded and waters are shown as spheres. The ion's hydrogen bonding partners and bond distances, clockwise from Asp264, are 2.94 Å and 2.49 Å, Asn460 (2.66 Å), Ser22 10 (2.57 Å), Gly20 (2.30 Å), and Phe260 (2.64 Å).

Figure 5 shows a ribbon diagram of one IMPDH monomer looking down the barrel of the protein with bound, XMP, NAD+ (both in CPK), and the potassium ion.

Figure 6 shows binding of the inhibitor MOA to IMPDH showing bonds (a) with IMP (substrate) and (b) with XMP (product). A notable difference is the movement of the Glu431 side chain, which binds both the substrate and the inhibitor in the IMP-bound structure.

Figure 7 shows a comparison of the active site loop of the B. burgdorferi apo structure (purple) with those of T. foetus IMP-bound (yellow), IMP+MPA (blue), XMP+MPA (green), and XMP+NAD+ (red) shows a high degree of stability throughout the core domain of the enzyme as well as the resolved portion of active site flap during substrate and product binding. Also pictured are XMP and NAD^+ in CPK and the potassium ion in gray.

Figure 8 shows a comparison of the fit of the T. foetus product XMP and NAD $^+$ into electron density. On the left, the T. foetus structure is shown with a 2Fo - Fc electron density map contoured at 1.0 σ , and on the right, the published human structure with 6-Cl IMP and the cofactor analog, SAD, uses a σ A-weighted Fo-Fc omit map. Panel b illustrates the binding of NAD $^+$ to the cofactor binding site of T. foetus IMPDH. NAD $^+$ makes extensive use of hydrogen bonds with IMPDH and ordered waters. The nicotinamide ring π -bonds with the purine ring of XMP while the adenosine ring stacks between Trp269 and Arg241.

figure 9 shows a structural alignment

demonstrates that potassium binding is conserved through all T. foetus structures presented here. The carbon atoms of a neighboring monomer are shown in dark gray. The T. foetus structure contains an aspartate at 264 while the mammalian enzyme (purple oxygens) has substituted a glutamine (b) and the bacterial enzyme (also purple oxygens) substitutes a histidine (c). Both of these side chains leave no room for the ion. An alignment of the T. foetus structure (blue), human structure (yellow) and S. pyogenes structure (green)

shows that this does not appear to uniquely alter the dimer interface (d).

Figure 10 shows a 2Fo-Fc electron density map contoured at 0.6 σ reveals that Π stacking is involved in forming the crystallographic dimer interface and that Trp416 from each monomer may occupy a position at the two-fold interface at 50% occupancy.

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Figure 11 shows structural formulas of the indicated compounds. The product XMP contains an additional keto group at the C2 position of the substrate IMP. This figure was created with Ligplot (Wallace et al., Prot. Eng. 8:127-134 (1995)) and Photoshop (Adobe Systems, San Jose, CA).

Figure 12 shows a Michaelis-Menten graph. The initial velocity increases with increasing concentration of substrate. The concentrations of enzyme and cofactor were held constant.

Figure 13 is a plot showing IMPDH inhibition

with increasing concentration of RMP. The concentrations of IMP, NAD⁺, and enzyme are constant.

Figure 14 shows a ribbon diagram of the IMPDH tetramer viewed looking down the four fold axis. The enzyme is in complex with the inhibitor RMP (CPK) and a sodium ion (green). A potassium ion (blue) lies in the dimer interface near the cofactor binding site. This image was made in Deepview (Guex and Peitsch, Electrophoresis 18:2714-2723 (1997)) and rendered in POVRAY 3.5 beta (www.povray.org).

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Figure 15 shows composite annealed omit electron density maps at 1.9 Å resolution surrounding the inhibitor RMP (a) contoured at 1.8 σ . The MOA-soaked RMP co-crystal structure (b) at 2.2 Å shows nearly complete density for MOA only when contoured at 0.5 σ despite

soaking in saturating amounts of MOA. Soaking for longer periods did not improve occupancy.

Figure 16 shows a diagram of RMP hydrogen bonds

with IMPDH. Like IMP, RMP makes many bonds with ordered
waters and main chain atoms. Only the Tyr405 hydroxyl
and the Asp358 carboxylate side chains make contact with
the inhibitor. Additionally, Met59, Ile318, and Gly407
make hydrophobic contacts. Solvent accessibility is
indicated by the yellow border around RMP, where lighter
color indicates greater accessibility. This figure was
created with NACCESS (Hubbard and Thornton, University
College London, Department of Biochemistry and Molecular
Biology, (1993)), HBPLUS (McDonald and Thornton, J. Mol.

Biol. 238:777-793 (1994)), and LIGPLOT.

Figure 17 shows that the ion binding site (green) is composed of backbone carbonyls from the active site loop residues, including the active site cysteine, and residues from the C-terminus of the neighboring catalytic monomer (gray carbons).

DETAILED DESCRIPTION OF THE INVENTION

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This invention relates to cystalline compositions of Tritrichomonas foetus (T. foetus) inosine monophophate dehydrogenase (IMPDH) complexes with its natural substrate, product, cofactor and inhibitors. The invention further relates to the discovery of high resolution crystal structures of different complexes of IMPDH, including complexes with its substrate IMP; with

IMP and inhibitor mycophenolic acid (MPA); with inhibtor ribovirin; with MOA and ribovirin; with the product XMP and MOA; and with XMP and the cofactor NAD^+ .

As disclosed herein, six complexes of T. foetus 5 IMPDH bound with IMP, IMP+MPA, XMP+MPA, XMP+NAD+, ribavirin and ribavirin+MOA. In particular, the highresolution crystal structures of four T. foetus IMPDH complexes with substrate, cofactor, and inhibitors -- IMP, $XMP+NAD^{+}$, IMP+MPA, and XMP+MPA—represent the first T. foetus structures with a complete active site, the first IMPDH structure with the NAD^+ cofactor bound, and the first with MOA bound in addition to unreacted substrate, and product. As is described in Example IV, a novel monovalent cation bound at the dimer interface that is 15 likely unique to T. foetus and can contribute to the stability of the cofactor binding site. The active site cation appears to be present only in the covalent substrate-complex and conformations further along the catalytic cycle for most eukaryotic organisms, but it is already present in prokaryotic organisms upon substrate binding.

Current development of drugs that bind IMPDH

has focused on developing highly potent inhibitors of the
human form of the enzyme. The invention provides
structural information useful for development of
inhibitors of microbial IMPDH. Compounds designed as
inhibitors of microbial IMPDH are useful for treating
diseases caused by a variety of microbes, including for
example, bacteria, viruses and parasites.

In one embodiment, the invention provides atomic coordinates for the bound complex of *T. foetus* inosine monophosphate dehydrogenase (IMPDH) with inosine monophosphate (IMP). The atomic coordinates for the IMPDH-IMP complex are provided in Table 2.

In another embodiment, the invention provides atomic coordinates for the bound complex of *T. foetus*IMPDH with IMP and mycophenolic acid (also referred to herein as MOA or MOA). The atomic coordinates for the IMPDH-IMP-MOA ternary complex are provided in Table 3.

In a further embodiment, this invention further provides atomic coordinates for the bound complex of T. foetus IMPDH with xanthosine monophosphate (XMP) and MOA. The atomic coordinates for the IMPDH-XMP-MOA ternary complex are provided in Table 4.

Also provided by the invention are atomic coordinates for the bound complex of *T. foetus* IMPDH with xanthosine monophosphate (XMP) and nicotinic adenine dinucleotide (NAD). The atomic coordinates for the IMPDH-XMP-NAD ternary complex are provided in Table 5.

The invention further provides atomic coordinates for the bound complex of T. foetus IMPDH with ribovirin (1- β -D-ribofuranosyl-1,2,4-triazole-3-carboxamide. The atomic coordinates for the IMPDH-ribovirin complex are provided in Table 7.

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The invention further provides atomic coordinates for the bound complex of *T. foetus* IMPDH with

above.

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Alternatively, modifications in the crystal
structure due to mutations, additions, substitutions, and
or deletions of amino acids; or other changes in any of
 the components that make up the crystal could also
  account for variations in structure coordinates.
   variations are within an acceptable standard error as
    compared to the original coordinates!
     three-dimensional shape is considered to be the same.
                The atomic coordinates of the invention can be
        stored in a memory or computer readable medium.
         or computer readable medium can be a hard disk!
          disc. compact disc. magneto-optical disc. Random Access
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          Memory Read Only Memory or Flash Memory and the like.
           computer system that contains the memory or computer
            readable medium used in the invention can be a single
             computer or multiple computers distributed in a network.
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                        The atomic coordinates of the invention are
                useful for viewing or manipulating the structure of IMPDH
                 in a conformation that binds IMP, XMP, MOA, NAD,
                  ribavirin, and combinations thereof. The atomic
                   coordinates shown in Tables 2-7 can be readily modified
                    to remove one or more atoms in the structure including
                     for example, the atomic coordinates for IMP, XMP, MOA,
                     NAD ribavirin
                       a portion of the structure is viewed or manipulated.
                       Other portions of the structures represented in Tables 2
                        That are useful in the invention include atoms of IMPDH
                         that interact with IMP, MOA, MAD or ribavirin, such
                          as those present in the active site loop! active site
                           flap, or in other residues that interact with the ligands
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as described herein; IMP or atoms thereof that interact with IMPDH; XMP or atoms thereof that interact with IMPDH; NAD or atoms thereof that interact with IMPDH; MOA or atoms thereof that interact with IMPDH; ribavirin or atoms thereof that interact with IMPDH. A portion of the atomic coordinates useful in the invention need not be a contiguous fragment of IMPDH or its bound ligands. The atomic coordinates can be manipulated or structures viewed on any computer that supports molecular modeling software such as a personal computer, silicon graphics workstation or super computer.

Portions of IMPDH or its bound ligands can be represented as pharmacophores. As used herein the term "pharmacophore" is intended to mean a representation of relative position for two or more atoms based on their positions in a molecular structure. In addition to relative position a pharmacophore can represent other characteristics of the atoms including, for example, charge or hydrophobicity. A representation in a pharmacophore can be a point indicating, for example, the center of the atom or the representation can be a volume indicating, for example, an area in which the atom can reside making a favorable interaction with another atom. A pharmacophore can also include a volume representing locations where an atom is disallowed, for example, due to unfavorable interactions with another atom.

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The atomic coordinates of the invention can be used in a variety of methods for rational drug design, such as in methods for identifying an inhibitor of IMPDH. Thus, the invention provides a method of identifying an

inhibitor of IMPDH. The method includes steps of: (a) displaying a structure for IMPDH, or a portion thereof, wherein the structure has atomic coordinates shown in Tables 2-7; (b) docking a structure of a candidate inhibitor to the structure of IMPDH, or the portion thereof; and (c) identifying an inhibitor of IMPDH, wherein the inhibitor has a structure that docks favorably to the structure of IMPDH, or the portion thereof. A structure of IMPDH can be represented with a pharmacophore of an IMPDH binding site.

As used herein, the term "docking" means a computational means for performing a fitting operation between the candidate inhibitor and a portion of the structure of IMPDH. Such a portion of the structure of IMPDH can be, for example, a binding pocket.

In one embodiment, the method is used to identify an inhibitor that targets the substrate binding site to which IMP or XMP bind. Accordingly, the method can be used with a portion of IMPDH that includes atoms that interact with IMP or XMP such as those described in Examples IV and VII. The method can also be used to identify an inhibitor that targets the NAD cofactor binding site to which NAD or MOA bind. A portion of IMPDH that interacts with MOA and that is useful in a method of the invention can include, for example, atoms that interact with NAD or MOA as described in Examples V and VII. Any portion of the IMPDH structures including, for example, the active site loop, active site flap or others described herein can be used in a method of the invention.

A structure of a candidate inhibitor can be docked to a binding site of IMPDH to identify an inhibitor that is complementary in shape to the binding site or has favorable electrostatic interactions with the charged groups in the binding site. A candidate inhibitor can be identified based on structural similarity to IMP, XMP, NAD, MOA or ribavirin. For example, a molecular structure database such as the Cambridge Structure Database can be searched to identify molecules having a particular structural attribute of IMP, XMP, NAD, MOA or ribavirin or any other inhibitor that binds to IMPDH.

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In one embodiment, the method is used to 15 identify an inhibitor that targets the substrate binding site to which RIBAVIRIN binds. Accordingly, the method can be used with a portion of IMPDH that includes atoms that interact with RIBAVIRIN such as Ser317 hydroxyl, Tyr405 hydroxyl, main chain nitrogen of Ser317, main 20 chain nitrogen of Gly381, main chain nitrogen of Arg382, the carboxylate of Asp358, the side chain of Ile318, hydrogen of Glu408 or hydrogen of Gly409. The method can also be used to identify an inhibitor that targets the NAD cofactor binding site to which MOA binds. A portion 25 of IMPDH that interacts with MOA and that is useful in a method of the invention can include, for example, the carbonyl oxygen of Gly312, the amide nitrogen of Gly314 or the sulfhydryl of Cys319. Any portion of the IMPDH structures including, for example, the active site loop, 30 active site flap or others described herein can be used in a method of the invention.

A structure of a candidate ligand can be docked using algorithms available in the art including, for example, those available in the software applications DOCK (Kuntz et al., <u>J. Mol. Biol.</u> 161:269-288 (1982)) or INSIGHT98 (Molecular Simulations Inc., San Diego, CA). Methods for screening a structural database to identify molecules that bind to IMPDH are described, for example, in Luecke et al., Exp. Parasitology 87:203-211 (1997).

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An inhibitor that targets IMPDH can be designed to contain a moiety from a ligand that binds the substrate binding site of IMPDH and a moiety from a ligand that binds to the cofactor binding site of IMPDH. The moieties included in such an inhibitor can be portions of ligands that are bound in the structures disclosed herein or can be analogs of any portion of these ligands, so long as the portion or analog is capable of binding to IMPDH when present in the inhibitor. Accordingly, the moieties of an inhibitor so 20 designed will function as binding moieties. The binding moieties can be linked by a third moiety that is capable of taking on a conformation that places the binding moieties in relative orientations similar to those observed in a crystal structure disclosed herein such as those having coordinates set forth in Tables 2-7. As an example, hydroxyl groups on the ribose rings of XMP and NAD, when bound in a ternary complex with IMPDH, both interact with aspartate residues of IMPDH. In particular Asp358 binds to the ribose hydroxyl of IMP or XMP and 30 ASP261 binds to the NAD(H) nicotinamide ribose hydroxyls as shown in Figure 10. The two aspartate residues are

about 6.5 angstroms apart at the closest point as shown in Figure 10. Accordingly, an inhibitor can be designed having two ribose moieties, or analogs thereof, linked to each other such that they can attain a conformation where they interact with these aspartates in IMPDH.

A method of the invention can further include a step of docking a candidate inhibitor to a second IMPDH structure. A second IMPDH structure used in a method of the invention can be a different conformation of the same IMPDH obtained, for example, by binding to different ligands. As described herein, the conformation of T. foetus IMPDH differs for the complexes described herein. Furthermore there are differences between the conformations of IMPDH disclosed herein and those for IMPDH bound to ribavirin phosphate and for IMPDH structures known in the art as set forth herein. Comparison of docking results for two or more different IMPDH conformations can be used to identify an inhibitor that has favorable binding interactions with IMPDH in multiple conformations. As described herein, the conformation of T. foetus IMPDH in a IMPDH-ribavirin complex differs from its conformation in an IMPDH-ribavirin -MOA ternary complex. Furthermore, the conformation of T. foetus IMPDH in a IMPDH-ribavirin complex differs from its conformation in apo IMPDH, IMPDH-IMP complex, IMPDH-XMP, IMPDH-XMP-MOA ternary complex, or IMPDH-XMP-NAD ternary complex. Comparison of docking results for two or more different IMPDH conformations can be used to identify an inhibitor that 30 has favorable binding interactions with IMPDH in multiple conformations. A structure of apo IMPDH is available in

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the protein databank (PDB) under PDB code 1AK5. A structures of IMPDH bound to ribavirin phosphate and a structure of IMPDH bound to ribavirin and MOA in a ternary complex are described herein.

aspects of IMPDH structure and association with substrate, products and inhibitors previously unrecognized. Based on particular structural features revealed, an inhibitor of IMPDH activity can be designed. Therefore, in one embodiment, the invention provides a method of the invention for identifying an inhibitor of IMPDH can involve displaying a structure for the bound complex of T. foetus IMPDH with NAD set forth in Table 5; (b) docking a structure of a candidate inhibitor to said structure, or the portion thereof; and (c) identifying a compound that binds Asp-358 and Asp-261, wherein said compound has a structure that docks favorably to said structure, or portion thereof.

A second IMPDH structure used in a method of the invention can be from a different organism. By comparing docking interactions for a candidate inhibitor with IMPDH from different organisms, an inhibitor can be identified that is specific for a particular organism. For example, an inhibitor that is specific to *T. foetus* IMPDH compared to IMPDH from a mammal can be identified based on favorable docking of the candidate inhibitor to *T. foetus* IMPDH and less favorable or even unfavorable docking with IMPDH from the mammal. Such an inhibitor can be useful as a therapeutic agent to treat a cow infected with *T. foetus* as set forth below.

Alternatively, comparison of docking results for IMPDH structures from two or more different organisms can be used to identify an inhibitor that has favorable docking with multiple IMPDH proteins, thereby identifying an inhibitor having relatively broad specificity. 5 Structures for IMPDH from other organisms that are useful in the invention include, but are not limited to, those for IMPDH from mammals including, for example, humans, primates, non-human primates, Chinese hamster, agricultural animals such as cow, horse, sheep, goats, 10 pigs; invertebrates, yeast, bacteria, or protozoa. Examples of IMPDH structures from other organisms that are useful in the invention include human type II IMPDH in a ternary complex with 6-Cl-Imp and selenazole adenine dinucleotide (PDB code 1B30); IMPDH from S. pyogenes (PDB 15 code 1ZFJ) and Chinese hamster IMPDH in complex with MOA (PDB code 1Jr1).

The invention provides another method of

identifying an inhibitor of IMPDH. The method involves

(a) selecting a candidate compound by performing

rational drug design with a set of atomic coordinates set
forth in Tables 2-7, wherein said selecting is performed

in conjunction with computer modeling; (b) contacting

said compound with IMPDH, and (c) determining the ability
of said compound to reduce IMPDH activity, wherein a
compound that reduces IMPDH activity is an inhibitor of
IMPDH.

The ability of a compound to reduce IMPDH activity can be determined using a variety of well known methods. Such methods include those described in Metz et

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al. Endocrinology 142:193-204 (2001) and Wilson et al. J. Biol. Chem. 266(3):1665-1671 (1991). Computer modeling can be performed using a variety of well known methods, including commercial modeling packages, such as those described herein above.

It is understood that the atomic coordinates of IMPDH disclosed herein can also be used for identifying a compound that increases the activity of IMPDH. Such a compound can be useful, for example, for increasing the viability of a microbe or as a therapeutic agent used to treat a disease or condition that is mediated by IMPDH or that can be reduced by increasing IMPDH activity.

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An IMPDH inhibitor identified by a method of the invention can be used as a therapeutic agent. A therapeutic agent identified using the methods of the invention can be used to treat a disease or condition that is mediated by IMPDH or that is reduced by inhibitors of this enzyme such as ribavirin or MOA. Such an agent can be used to treat a mammal, agricultural animal, human, dog, cat or horse. For example, an inhibitor of T. foetus IMPDH can be used to treat cows infected with the T. foetus protozoan. A therapeutic agent identified using the methods of the invention can be used as an antiproliferative, antiviral, anticancer or immunosuppresive agent. A therapeutic agent identified using a method of the invention can be useful for treating a cancer such as those causing a benign or malignant tumor of the breast, prostate, colon, lung, brain or ovary. A therapeutic agent identified using a method of the invention can be useful for treating a

viral infection such as one caused by hepatitis A, B or C; respiratory syncytial virus, HIV or hanta virus. therapeutic agent identified using a method of the invention can be useful for treating a fungal infection such as one caused by Aspergillus, Penicillium, Alternaria, Cladosporium, and Fusarium. A therapeutic agent identified using a method fungal viral infection such as one caused by Aspergillus, Penicillium, Alternaria, Cladosporium, and Fusarium. A therapeutic 10 agent identified using a method of the invention can be useful for treating a bacterial infection such as one caused by Staphylococcus spp., Streptococcus spp., Haemophilus influenzae, Pseudomonas aeruginosa, enteric Gram-negative bacilli, Moraxella lacunata, Acinetobacter spp., Neisseria gonorrhoeae, Branhamella catarrhalis, 15 Clamydia trachomatis, and anaerobes. A therapeutic agent identified using a method of the invention can be useful for treating a parasitic infection such as one caused by Acanthamoeba and Toxoplasma gondii. A therapeutic agent 20 identified using a method of the invention can be useful in combination with other treatments, for example, as an immunosuppressive agent administered following organ or cell transplantation.

It is understood that modifications which do not substantially affect the activity of the various embodiments of this invention are also included within the definition of the invention provided herein.

Accordingly, the following examples are intended to illustrate but not limit the present invention.

EXAMPLE I

Cystallization of *T. foetus* IMPDH with Bound Substrate, Cofactor and Analogs

This example shows expression, purification, and crystallization of T. foetus IMPDH with bound IMP, IMP+MPA, XMP+MPA, and XMP+NAD $^{+}$.

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Protein expression and subsequent purification yielded approximately 90 mg of pure and active protein as determined by Coomassie stained SDS PAGE gels and a spectrophotometrically observed increase of NADH when enzyme is added to IMP and NAD+ using previously described methods (Digits and Hedstrom, Biochem. 38:2295-2306 (1999)). This yield could be increased substantially by optimizing the fermentation parameters, in particular by supplementing oxygen, as this was the limiting factor.

Parasitol. 63:221-229 (1994)) containing T. foetus IMPDH (Beck et al., Exp. Parsitol. 78:101-112 (1994)) was transformed into Escherichia coli strain H712 (E. coli Stock Center, Yale University, New Haven, CT). This bacterial strain is deficient in native IMPDH and requires rich media for growth unless supplemented with a source of GMP or guanosine. Expression of T. foetus IMPDH was achieved by activation of the PhoA promoter under low phosphate conditions using supplemented MOPS minimal media using a modified version of previously

published protocols (Craig et al., <u>Proc. Natl. Acad. Sci. USA</u> 88:2500-2504 (1991); Neidhardt et al., <u>J. Bacteriol.</u>
119:736-747 (1974); Yuan et al., <u>J. Biol. Chem.</u>
265:13528-13532 (1990)). Briefly, the cells were grown in MOPS media in a 19-liter fermentor (Wheaton Science Products, Millville, NJ.) inoculated with 0.5 liters of overnight MOPS culture of H712 containing the IMPDH plasmid. Temperature was maintained at 37° C, dissolved oxygen (DO) was maintained at greater than 40% with aeration, stirring, and glucose addition. The cells were harvested at 8 hours when the DO dropped to below 20% at roughly OD600 = 1.5.

The cells were concentrated to 0.5 L by 15 tangential flow filtration (Millipore, Inc., Bedford, Ma.), pelleted by centrifugation at 6,000 g, then resuspended in a three fold volume of buffer A (50 mM Tris pH 8, 50 mM KCl, 10% glycerol, and 1 mM 2mercaptoethanol) supplemented with protease inhibitors and 1 mM EDTA. The cells were then flash frozen in 20 liquid nitrogen before storage at ~85° C. This mixture was lysed by French Press and clarified by centrifugation at 20,000 g. The resulting lysate was then run over a Cibacron blue column on an AKTA FPLC (Amersham-Pharmacia). Cibacron blue is a dye ligand that 25 selectively binds many proteins that use NAD as a cofactor. The protein was found to elute from the column in a broad peak with a gradient of 50 mM - 1M KCl over 20 column volumes. Protein elution from the column was optimized by eliminating the gradient and eluting the 30 protein in 1 M KCl. This was followed by dialysis into buffer A and concentration to 15 mg/ml. The protein was

then passed through a monoQ column (Amersham-Pharmacia) using a gradient from 50 mM to 500 mM KCl over 20 column volumes. The resulting protein was >90% pure and was dialyzed in buffer A and concentrated to 30 mg/ml for storage at -85° C.

The protein was first crystallized by optimizing previously published conditions (Whitby et al., Proteins 36:10666-10674 (1995)) by mixing 10-15 mg/ml protein in buffer A into 2.4 M ammonium sulfate, 100 mM Tris pH 8.0, 10% glycerol, 4 mM PEG 400, and 1 mM 2-mercaptoethanol well solution in 6 µl sitting drops in a 1:1 ratio of well solution to protein at 20° C. Crystals diffracting to higher resolution were obtained with the substitution of 42% saturated sodium malonate for 2.4 M ammonium sulfate. Additionally, the crystals grew to a larger size without increased mosaicity, and the malonate provided excellent cryo-protection as no other additives were necessary.

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EXAMPLE II

Crystalography Data Collection for of T. foetus IMPDH Complexes

This example describes data collection for T. foetus IMPDH crystal structures with bound IMP, IMP+MPA, XMP+MPA, and XMP+NAD $^{+}$.

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All of the ligands were co-crystallized with the exception of NAD^{\dagger} and XMP. In the $NAD^{\dagger} + XMP$ structure,

the NAD^+ and XMP were added to five to seven day old crystals and allowed to soak for five days before data collection. Attempts were made to generate XMP covalently attached to the active site cysteine (E-XMP*) by addition of IMP to IMPDH in a reaction buffer containing NAD+ and MOA using methods previously described. The resulting x-ray structure was identical to the XMP+MPA co-crystal structure: there was clearly an oxygen atom on the C2 of XMP, but no covalent bond with the active site cysteine could be discerned.

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Diffraction quality crystals grew within five days and although the crystal morphology changed due to the substitution of malonate for sulfate, the space group remained P432 (Figure 1). The cryo-frozen crystals diffracted from 1.95 to 2.2 Å using synchrotron radiation. A randomly selected test set of diffraction data (5% of all structure factors) was set aside for Rfree calculations. All model building was carried out with the program O, and the program CNS was used for refinement. The original T. foetus apo structure was used as the initial model for all structures allowing unbiased building of the active site loop and flap. One round of rigid body refinement and simulated annealing was followed by several rounds of energy minimization, B factor refinement, model building, and water picking. Composite omit, $2F_o-F_c$, and F_o-F_c maps were generated to The program PROCHECK was used to quide model building. validate the structures (Laskowski et al., J. App. Cryst. 26:283-291 (1993)). Crystal, refinement, and PROCHECK 30 statistics are presented in Table 1.

Initial diffraction of T. foetus IMPDH using the published ammonium sulfate crystallization conditions only reached 3.2 Å using a RAXIS IV detector. modified conditions improved resolution to 2.45 and resolution was further improved using synchrotron radiation. Synchrotron data were collected at the Stanford Synchrotron radiation laboratory (SSRL) beam line 9-1 and at The Advanced Light Source, Lawrence Berkeley National Laboratory (ALS) beam line 5.0.2. Xray data collection, reduction and refinement statistics 10 can be found in Table 1. Diffraction data were collected under cryo conditions using colorless crystals ranging in size from 0.4 to 0.8 mm. The crystals were loop-mounted and flash-cooled to -170° C in the nitrogen stream. data were collected from single crystals and integrated 15 and scaled in the Denzo-Scalepack package (Otwinowski, Data Collection and Processing, SERC Daresbury Laboratory, Warrington, UK, pp. 56-62 (1993)). The published apo structure (Whitby et al., Biochem. 36:10666-10674 (1997)) was used as an initial model for 20 all co-crystals, followed by rigid body and simulated annealing refinement. Several rounds of model building, energy minimization and B-factor refinement were then performed with the programs O (Jones et al., Acta Cryst. A47:110-119 (1991)) and CNS (Brunger et al., Akta Cyrst. 25 D54:905-921 (1998)).

EXAMPLE III

Model Building for T. foetus IMPDH with bound IMP, IMP+MPA, XMP+MPA, and XMP+NAD⁺

This example describes model building for T. foetus IMPDH with bound IMP, IMP+MPA, XMP+MPA, and $XMP+NAD^{+}$.

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All IMPDH are homotetramers in solution under physiological conditions. In the cubic P432 spacegroup, this catalytic tetramer is formed by the crystallographic four-fold axis (Figure 2). The active site loop, residues 313-330, was modeled in all but the XMP+NAD+ bound structure, which lacks residues 318-321. This loop is highly mobile, in part due to three glycine residues (residues 314-316) near the active site cysteine. Additionally, this loop has not been stabilized by covalently binding a substrate intermediate or inhibitor, resulting in weak electron density and high B factors. Visualization using electron density maps at lower contouring levels (0.5-0.8 g) resulted in continuous or nearly continuous density throughout backbone of the active site loop (Figure 3) with the exception of the NAD⁺ structure.

Furthermore, a larger portion of the active site flap (residues 408-433) was ordered in these structures in comparison to previous *T. foetus* structures. However, the distal portion of this loop was not modeled. Although there was scattered density for

the 120-residue CBS domain, it was not contiguous and despite the improved resolution, this domain was not included in the model. Only the *S. pyogenes* structure contains the entire CBS domain (Zhang et al., <u>Biochem.</u> 38:4691-4700 (1999)).

The substrate IMP, product XMP, cofactor NAD+, and inhibitor MOA hetero-atoms in the structures presented here were placed into the apo model only when positive density was observed in Fo-Fc, 2Fo-Fc, and composite omit maps. The XMP was taken from the original T. foetus XMP structure (Whitby et al., supra, (1997)) and the IMP model was derived from this XMP structure. The NAD model was obtained from the phosphoglycerate dehydrogenase structure (Schuller et al., Nat. Struct. Biol. 2:69-76 (1995)) and the MOA model from the Chinese hamster IMPDH structure (Sintchak et al., Cell 85:921-930 (1996)). The IMP, XMP, and MOA hetero-atoms were fitted into density using O and minimized in CNS. coordinates for NAD+ were fitted as above and subsequently submitted to the Dundee PRODRG Server (van Aalten et al., J. of Computer Aided Mol. Design 10:255-262 (1996)) for minimization and CNS topology file generation prior to refinement in CNS.

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A cis peptide bond not previously described for IMPDH was located in all structures between Gly290 and Asn291 and is located within 7 Å of the nicotinamide portion of the NAD⁺ cofactor. This was present but not described in the *T. foetus* model co-crystallized with XMP (Whitby et al., *supra*, (1997)) but absent in all other structures to date. The cis bond appears to cause the

chain to turn away from the active site, preventing it from entering the active site. All other IMPDH x-ray structures have this same turn but a cis peptide has not been reported in those structures.

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A novel potassium ion was also identified in all structures, approximately 9 Å away from the cis peptide. This ion is coordinated by the backbone carbonyl of Phe266, the side chain carboxyl oxygens of Asp264, and the following atoms of a neighboring monomer: backbone carbonyls of Gly20 and Asn420, and the Ser22 hydroxyl oxygen (Figure 4). The potassium ion also lies near the NAD⁺ binding site and appears to stabilize the monomer-monomer interface as well as the cofactor binding site, but it does not make direct contact with NAD⁺ (Figure 5).

A strong electron density peak was found extending from the active site cysteine thyol in the IMP and IMP+MPA bound structures. This appears to be a result of oxidation to sulfenic acid (Cys-SOH) from oxygen exposure during crystal formation and extended incubation prior to cryo-cooling for data collection. This type of oxidation has been previously described for NADH peroxidase (Stehle et al., <u>J. Mol. Biol.</u> 221:1325-1344 (1991)). Although it is interesting that the cysteine was modified only in the IMP-bound structures, this could be an artifact of crystallization as the active site cysteine was not resolved in the XMP+NAD structure, and the XMP+MPA structure had poor density around the cysteine.

EXAMPLE IV

Substrate and Product Binding to T. foetus IMPDH

This examples describes substrate and product binding to *T. foetus* IMPDH.

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In all complex structures presented herein, the substrate/product sugar hydroxyls are hydrogen bonded to the carboxyl side chain of Asp358 as well as two waters. The purine O6 accepts a hydrogen-bond from the amide nitrogens of Glu408 and Gly409. The side chain of Ile318 makes van der Waals contact with the base. The nucleotide phosphate group is coordinated by the hydroxyl of Tyr405, backbone nitrogens of Ser317 Gly381, and Arg382, and three waters.

In the IMP complex structure, the purine N1 and N3 both form hydrogen bonds with waters. The water in contact with N1 is bridging it to the backbone carbonyl of Glu431, which is 4.79 Å from the N1 as well as Gln324. This portion of the active site flap was modeled into relatively poor density but the water is clearly observed, as well as the backbone from residue 429-431. The water on N3 is bridging it to the backbone nitrogen of Gly316. The phosphate group is coordinated by the hydroxyl and the main chain nitrogen of Ser317. The IMP+MPA complex differs from the IMP structure in that the purine N1 is forming a direct hydrogen bond with the Glu431 carboxylate oxygen. The other Glu431 carboxylate oxygen is in contact with the MOA ring hydroxyl.

Only in the XMP+MPA structure is the backbone carboxyl of Glu431 in direct contact with N1 and the active site flap is not shifted in this structure. The XMP+NAD+ complex structure is also characterized by the backbone carbonyl of Glu431 in direct contact with the purine N1. As in the IMP bound structure, the hydroxyl of Ser317 is pointing toward the XMP phosphate. However, the main chain nitrogen of Ser317, which was coordinating the water hydrogen bonding with N3 in the IMP structure, has moved 0.37Å further away from the substrate and the water is no longer present.

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Binding in the substrate-binding pocket is characterized by subtle conformational changes when binding IMP vs. XMP. Furthermore, a comparison with other IMPDH structures reveals few changes to the active site across species. IMP binds to the S. pyogenes enzyme in a nearly identical fashion as it binds to the T. foetus enzyme. Most noticeably, the purine ring system of the S. pyogenes IMP is rotated away from the catalytic In T. foetus IMPDH, the ring system does not rotate away. Instead, it is the active site Cys319 that is displaced 1.3 Å from the catalytically active conformation. A structural alignment of T. foetus, S. pyogenes, and Chinese hamster IMPDH shows that the active site loops are almost identically positioned. Based on surrounding charges, bond distances, and geometry, we believe that there is a cation present in the bacterial structure at the position marked as water 179 in the coordinate entry (Zhang et al., supra, (1999)). Because the active site cysteine is displaced in the IMP-bound structure of the protist, the Cys319 backbone carbonyl

disrupts the ion binding pocket. In the *T. foetus*XMP+MPA structure, the XMP C2 keto group causes the active site cysteine to move even further into the cation binding pocket.

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Human type II IMPDH has the T. foetus Lys310 and Glu431 substituted with arginine and glutamine, accounting for part of the difference in sensitivity to MOA (Digits and Hedstrom, supra, (1999)). located near the N1 nitrogen of the IMP. structures presented here, only the IMP+MPA structure shows the side chain interacting with partially positively charged groups on both the IMP and MOA rings. In the other T. foetus structures, as well as the Chinese hamster and human type II structures, Glu431 is pointed away from the IMP, and toward the MOA or SAD inhibitors, leaving the main chain carbonyl pointed at the IMP, XMP, or 6-Cl IMP. The hamster Gln441 side chain is within hydrogen bonding distance of the MOA ring hydroxyl. lysine or corresponding arginine is pointing between the IMP sugar hydroxyls and the MOA or cofactor. Because the arginine side chain is longer, they are near hydrogen bonding distance with one of the ribose hydroxyls of IMP and near the methyl group on the MOA ring.

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RMS alignments of the substrate and product complex structures show very little movement in the core of the protein as well as the ordered portions of the active site flap. Unfortunately, the structures presented here have 10 to 14 residues missing from the active site flap, making characterization difficult. A possible explanation for this disorder is described

below. The majority of conformational differences are located at the active site loop. The active site loop was resolved in all structures with the exception of the NAD⁺XMP co-crystal. In all cases, the loop is not well ordered with high B-factors, but overall, little movement is observed in the protein backbone of these structures with the exception of the IMP+MPA complex.

In the IMP+MPA structure, the side chains of 10 'the active site flap residues 431 to 434 move away from the active site to allow Glu431 to rotate around the $C\alpha$ -Cmain chain bond and form hydrogen bonds with the IMP N1 and the MOA ring hydroxyl. The active site loop residues 320 to 323 shift away from the substrate+inhibitor complex with the Arg322 alpha carbon moving 7.5 Å from 15 its position in the XMP+MPA model. It is unclear from these structures what is driving this movement of the loop, as these residues do not appear to be directly involved in substrate or cofactor binding. The nearest of these residues, Thr321, is 6.6 Å away from the MOA in 20 the XMP+MPA structure. This complex is unlikely to occur under physiological conditions since NAD has a far greater binding affinity than MOA. However, MOA does make a useful cofactor analog for the nicotinamide portion of the NAD binding site. This unique pairing may be useful in structure based drug design since a structure containing unreacted substrate and cofactor may be more difficult to obtain.

EXAMPLE IV

Cofactor and Inhibitor Binding to T. foetus IMPDH

This example describes cofactor and inhibitor binding to *T. foetus* IMPDH.

In the two MOA complex structures (IMP+MPA and XMP+MPA), the inhibitor is bound in a similar manner (Figure 6a and b). One difference, however, is that the 10 side chain of Glu431, which is hydrogen bonding with both the IMP and MOA, is shifted away from the productinhibitor complex in the XMP+MPA structure. This may be caused by the stronger partial negative charge on the XMP due to the keto group at the C2 position of the base. The main chain nitrogen of Gly314 has moved from 3.26 Å to 3.64 Å away from the MOA ring O1. The nicotinamide portion of the NAD cofactor stacks with the XMP purine moiety and the nicotinamide oxygen hydrogen-bonds with the Gly314 nitrogen in the same manner as the MOA 20 inhibitor. Additionally, the nicotinamide phosphate forms bonds with the hydroxyls of Ser262 and Ser263, as well as the main chain nitrogen of Ser263. carboxylic acid tail of MOA also binds the Ser263 hydroxyl and nitrogen. The nicotinamide sugar hydroxyls form hydrogen bonds with Asp261. The NAD adenosine ring 25 stacks between the side chains of Trp269 and Arg241. Arg241 also forms hydrogen bonds with the adenosine phosphate group.

30 Shown herein is the first IMPDH structure with both the XMP product and the NAD cofactor bound.

Although the human type II structure has 6-Cl IMP and the

NAD analog SAD bound in the respective substrate and cofactor binding sites, the 2.9 Å structure left some ambiguity in the positioning of the SAD molecule (Colby et al., Proc. Natl. Acad. Sci. USA 96:3531-3536 (1999)). At 2.15 Å and with good electron density in the cofactor binding site, we were able to accurately place the cofactor (Figure 8). Although the cofactor lies near the monomer-monomer interface, it does not make contact with the neighboring subunit in the T. foetus tetramer. nearest residue is Ile27, 4.7 Å away from the adenosine 10 portion of the cofactor. This is in contrast to the human structure where the neighboring monomer makes contact with the adenosine ring. The nicotinamide sugar hydroxyls in the T. foetus structure form hydrogen bonds with Asp261 and two waters in the same manner as the substrate ribose hydroxyls interact with Asp358. Asp261 is completely conserved across species. In the human structure the cofactor sugar is further from the nicotinamide plane and one of its hydroxyls is out of reach of the human Asp274. 20

The proximal portion of the active site flap lies near the cofactor but the electron density is too ambiguous to discern any contacts. Similarly to the human type II structure, the adenosine portion of the cofactor is stacked between Arg241 and Trp269. These residues correspond to His253 and Phe282 of human type II IMPDH, and Arg253 and Tyr282 of human type I IMPDH. It is clear that this stacking is conserved in both the mammalian and T. foetus structures. Interestingly, the S. pyogenes model contains threonine and glycine in these positions, and with the exception of P. furious, which

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contains arginine and lysine residues, respectively, no bacterial sequence contains a stacking partner for the IMPDH cofactor at this location. This suggests that bacterial enzymes may have an alternate cofactor binding mechanism and may be the reason why the bacterial enzyme has a lower affinity for NAD⁺. If the NAD⁺ adenosine ring is indeed not involved in base stacking in the bacterial structure, an effective inhibitor may be a mononucleotide nicotinamide derivative.

MPA does not appear to trap the covalently bound product. The inhibitor MOA binds to IMPDH in the nicotinamide portion of the cofactor-binding pocket using many of the same binding partners as the cofactor. The cofactor NAD⁺ binds to IMPDH with many more interactions and therefore has a greater binding affinity to the enzyme when substrate is bound. Our failure to generate the covalent intermediate may be due to T. foetus IMPDH having a far faster release of E-XMP* than the mammalian enzyme (Digits and Hedstrom, supra, (1999)) or it may simply be that MOA does not inhibit XMP disassociation from T. foetus IMPDH. MOA does bind the T. foetus enzyme with significantly lower affinity than the mammalian form.

A novel potassium binding site was also identified. A high positive difference density peak in the F_o - F_c electron density map was observed at a dimer interface near the cofactor-binding site. This peak was surrounded by four backbone carbonyl oxygens and the carboxylate of Asp264 (Figure 4). The charge environment indicates a cation, and the coordination and B factor are

a probable indication of a potassium ion. This potassium is located too far from the substrate and cofactor to affect catalysis or to directly affect binding (Figure 5). However, it may aid in cofactor binding by stabilizing adjacent residues, which are involved in cofactor binding. Additionally, the monovalent cation likely stabilizes the dimer interface. This ion is present in all structures presented here (Figure 9a). The ion was not noted in the previous T. foetus structures (Whitby et al., supra, (1995); Whitby et al., supra, (1997)), but there was a water molecule placed at that location in the T. foetus XMP-bound structure. It is possible that the previous T. foetus structures were not at sufficient resolution to detect the ion.

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This ion appears to be unique to T. foetus IMPDH and is not likely to represent the second ion binding site proposed for the E. coli enzyme (Kerr et al., Arch. Biochem. Biophys. 375:131-137 (2000)). A protein alignment shows that the T. foetus Asp264 is substituted with glutamine in most eukaryotic IMPDH and with histidine in prokaryotic IMPDH. A structural alignment with the human and bacterial structures (Colby et al., supra, (1999); Zhang et al., supra, (1999)) shows that the substitutions would cause steric and charge clashes with the potassium (Figure 9 b and c). Absence of this ion does not appear to affect the secondary structure of either human or bacterial IMPDH (Figure 9d). The potassium ion reported in Chinese hamster IMPDH was not detected in these structures. This is likely due to the highly mobile nature of the active site loop that forms part of the T. foetus IMPDH potassium binding site.

bond between Ser83 and Gln84 (Figure 10). This tryptophan is physically able to fit in either position; however, residues 414 and 415, which also move as a result of the two conformations, have little density in either conformation and there is no usable density beyond Trp416 in either conformation. We believe that the residues beyond Trp416 are disordered, in part, because of the multiple conformations of this tryptophan. Mutation of this residue may aid in resolving this loop but it is also likely to inhibit crystallization due to the loss of this crystal contact. Furthermore, the tryptophan may be stabilizing the active site flap residues preceding it, and a mutation may cause a loss in resolution of a greater portion of the loop as is the case in most other IMPDH structures. It is possible that addition of adenosine or its analogs to this mutant protein could bridge the II systems of the two monomers, however this hypothesis has not been tested.

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EXAMPLE V

Proposed Structural Mechanism for T. foetus IMPDH

This example describes the proposed structural mechanism for T. foetus IMPDH.

An improvement upon the original *T. foetus* 2.3 Å apo structure structure showing the active site loop would increase the understanding of the catalytic mechanism of IMPDH. This is likely due to the increased flexibility of the *T. foetus* loop due to the three consecutive glycine residues present in the loop. The *T.*

foetus Gly315 is substituted with a proline in B. burgdorferi, likely providing the active site loop with increased stability. It appears that the T. foetus loop is stabilized only by occupation of the active site. If the apo T. foetus active site loop conformation is similar to that of the B. burgdorferi loop, a hypothesis of the IMPDH structural mechanism can begin to be described.

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The kinetic mechanism is random-in ordered-out with NADH leaving before XMP is released from the enzyme. When IMP binds the enzyme first, the enzyme is in an open conformation and IMP has easy access to the active site. When ${\rm NAD}^{\scriptscriptstyle +}$ binds first, the nicotinamide group blocks one entrance to the active site. Now, IMP must instead use the opening defined by the active site loop in its open configuration. An alignment of the apo B. burgdorferi structure and the T. foetus IMP-bound structure reveals an opening leading to the active site that is approximately 10 Å wide and 12 Å tall between the loop and the flap (Figure 11). This opening, together with the flexible nature of the loop and the flap, would allow access to the active site. Additionally, Ser317 and the hydrophobic Ile318 are solvent-exposed. These two amino acids may serve as a bait to draw IMP into the structure. When IMP binds in the active site, it causes the loop to close and Ser317 to bind to the phosphate, while the Ile318 side chain forms hydrophobic interactions with the purine ring. This, in effect, closes the lid, and the substrate IMP or the product XMP must wait for NADH to leave before either nucleotide can dissociate from the enzyme.

there are no active-site bonds present in the IMP structure that are not present in the product+inhibitor or product+cofactor structure. It appears that the enzyme relies on the release of the cofactor and subsequent solvent exposure of the product with its newly formed keto group and the corresponding partial negative charge, in order for product to be released. This observation confirms kinetic studies of the T. foetus enzyme that show the off-rate of IMP at 7.7 s-1 and that of XMP at 17 s-1 without cofactor bound (Digits and Hedstrom, supra, (1999)). Additionally, the nicotinamide ring of NADH would lie near the O2 carbonyl of the product XMP; this newly developed partial charge may act to push the now less polar ring out of the active pocket.

The identification of a cation at the active site of the Chinese hamster structure and the possibility of a cation in the same location in the S. pyogenes structure are intriguing. An ion present when the substrate is bound but unreacted and still present when product is covalently bound might indicate that this ion is important in placing the active site cysteine in an orientation required for catalysis.

In the bacterial structure, Thr310 makes hydrogen bonds with an ordered water and the Glu420 main chain. This creates a stabilizing effect for several residues in the loop as well as the C-terminal portion of the active site flap. Examination of the other bacterial structure, B. burgdorferi in the apo conformation,

reveals that the threonine is not in position to form bonds with the active site flap, resulting in a larger section of the C-terminal portion of the flap to be disordered. It appears that this increased stability in the S. pyogenes active site loop, and of Cys310 in particular, causes the purine to rotate away from the active site cysteine. In the T. foetus structure, Thr310 is substituted with Ile320 and this hydrophobic residue is likely to destabilize the active site loop in this conformation, allowing the cysteine to move rather than the purine. This threonine is conserved in prokaryotes while most eukaryotes carry the isoleucine. Apparently, it is the covalent bond with the substrate that is the stabilizing factor in the Chinese hamster model and it would not be surprising to find that the Ile-Thr substitution plays a role in prokaryote vs. eukaryotic enzyme kinetics.

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EXAMPLE VI

Steady State Kinetic Analysis of T. foetus IMPDH

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Steady-state kinetic analysis of to *T. foetus*IMPDH using IMP as a substrate was performed using a spectroscopic method. Initial velocity measurements were taken with increasing amounts of IMP and plotted as a Michaelis-Menten graph (Figure 12).

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From the plot, an apparent Km of 3.0 M was calculated for IMP. RMP, a competitive inhibitor for the

substrate IMP, was then assayed for inhibition of the protozoan enzyme with increasing concentrations of RMP. These data were graphed as a Dixon plot (Figure 13). The apparent Ki for RMP was determined to be 65 nM.

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Steady-state kinetic analysis of T. foetus IMPDH was performed with 4.5 M enzyme in a reaction buffer containing 100 mM KCL, 50 mM Tris pH 8.0, 1 mM DTT and 1 mM NAD+. Reactions were initiated with the addition of IMP, and the production of NADH was monitored spectrophotometrically at 340 nm (340 = 6.22 mM⁻¹ cm⁻¹) using a Perkin Elmer Lambda 40 (EG&G, Inc., Wellesley, Ma) spectrophotometer at 25°C. For determination of the apparent Km value for IMP, the concentration of IMP was varied from Km/2 to 10Km with the NAD concentration fixed at 1 mM. The initial velocity at various IMP concentrations was measured and was fit to the Michaelis-Menten equation by Sigma plot (SPSS Inc., Chicago, Il.). Since RMP is known to be a competitive inhibitor with IMP, the apparent inhibition constant Ki of RMP was estimated using a Dixon plot. In the experiments, RMP concentration was varied while IMP concentration remained fixed at 40 M, and the NAD concentration was 1 mM. initial velocities at various RMP concentrations were determined by the extraction of the linear portion of the reaction time-course. By plotting 1/v vs. inhibitor concentration, the apparent inhibition constant Ki was calculated using the following equation:

30 $1/v = (K_m/V_{max}) (K_i[IMP]) [RMP] + 1/V_{max} (1+(K_m/[IMP]))$

EXAMPLE VII

Crystallization to *T. foetus* IMPDH with Ribovirin

Diffraction quality IMPDH crystals in the space group P432 grew within five days. The cryo-colored crystals diffracted to 1.90 Å for the RMP co-crystal and to 2.15 Å for the crystal with RMP and MOA using synchrotron radiation. A randomly selected test set of diffraction data (5% of all structure factors) was set aside for Rfree monitoring. The published isomorphous T. foetus apo structure (PDB code 1AK5) was used as the initial model for both structures allowing unbiased building of the active site loop and the active site flap. One round of rigid body refinement and simulated annealing was followed by several rounds of energy minimization, B factor refinement, model building, and water picking. Composite 2Fo-Fc and Fo-Fc omit maps were generated to aid in model building. The program PROCHECK was used to validate the structures (Laskowski et al., J. App. Cryst. 26:283-291 (1993)). Crystal, refinement, and PROCHECK statistics are shown in Table 9.

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IMPDH crystallized as a homotetramer with monomers related by the four-fold crystallographic axis (Figure 14). The active site loop, residues 313-330, was modeled in both the RMP and RMP+MPA structures. The proximal portion of the active site flap (residues 408 to 416 and 431 to 433) was modeled, while the distal portion (residues 417-430) was disordered. Poor density in the

region of the CBS domain was observed and no attempts were made at modeling this domain. The C-terminal amino acids 484-492 were also added to the original T. foetus model and although these nine residues do not appear to make direct contact with substrate or product, they do lie near the active site of a neighboring monomer in the catalytic tetramer and the backbone carbonyls of residues 485-487 from part of the active site cation binding pocket. Although RMP was clearly observable in the electron density of both crystal structures, density for MOA, even with saturating concentrations in the crystallization drop, was weak and was therefore modeled at 50% occupancy (Figure 15). B factors for MOA at this level of occupancy were in agreement with the neighboring RMP atoms.

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A cis peptide bond was modeled in both structures between Gly290 and Asn291. It is located near the cofactor binding site but does not appear to be close enough to directly influence cofactor binding. In addition, a strong peak of electron density was found extending from the active site cysteine sulfur in the RMP bound structure. This appears to be a result of the thiol oxidized to sulfenic acid (Cys-SOH), likely caused by exposure to oxygen during crystal formation prior to freezing.

As was observed in the IMP bound structure, the phosphate is coordinated with hydroxyls from Ser317 and Tyr405 as well as main chain nitrogens from residues 317, 381, and 382 (Figure 16). Three solvent waters also form hydrogen bonds with the phosphate. As in all IMPDH

structures, the substrate sugar hydroxyls form strong hydrogen bonds with a conserved aspartate carboxylate (Asp358). Ile318, which in the substrate and product complexes forms hydrophobic interactions with the purine ring, has moved 1.2 Å away from the RMP inhibitor. The RMP amide oxygen forms hydrogen bonds with Glu408 and Gly409. In the RMP+MPA structure the amide nitrogen is hydrogen-bonding to the MOA ring hydroxyl and the MOA inhibitor has moved 0.6 Å from its position in the XMP+MPA structure in the direction of the RMP purine ring derivative. In this position, the MOA ring O2 makes a hydrogen bond with the backbone nitrogen of Gly314, and the C3 oxygen hydrogen bonds with the catalytic sulfhydryl of Cys319.

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The conformation of the active site loop in the RMP as well as the RMP+MPA structure is different from the loop conformation of the structures with bound substrate or product, resulting in a pocket surrounded by backbone carbonyl oxygens from Gly314, Gly316, and the active site Cys319, as well as carbonyls from Glu485, Gly486 and Gly487 in the neighboring catalytic monomer. A high (7.7 sigma) difference density peak was observed at the center of this pocket indicating the presence of a cation. Both Na+ and K+ ions were modeled into this site and minimized in CNS. A large peak of negative difference density was observed when K+ was modeled as well as high B factors. Because of the high concentration of sodium in the crystallization buffer, the previous observation that a sodium ion binds competitively with K+ in microbial IMPDH (Kerr et al., Arch. Biochem. Biophys. 375:131-137 (2000)), and B

factors that are near that of the neighboring atoms, a Na+ ion was placed in the final model (Figure 17).

As is described above, T. foetus IMPDH binds ribavirin in the active site substrate pocket. RMP+MPA complex was difficult to obtain, as the MOA inhibitor was only observed with saturating amounts of MOA present in the crystallization drop. Attempts to obtain a co-crystal rather than an MOA soak were unsuccessful as the levels of MOA necessary to form the complex inhibited crystal formation. Although no data have been reported on the additive effects of ribavirin and MOA, it is unlikely that both inhibitors would occupy the substrate and cofactor binding pockets of the active site simultaneously, despite their distinct binding The reason might be that MOA appears to rely on stacking its ring against the product XMP purine ring to bind to IMPDH and the RMP ring is probably too small for effective stacking.

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A structure of RMP bound to human IMPDH has not been made available for direct comparison; however, we were able to compare the *T. foetus* RMP structure with the Chinese hamster structure that contains a covalently bound substrate intermediate (Sintchak et al., supra, (1996)). These structures show a high degree of similarity in the conformation of the active site loop, recruitment of a catalytic ion, as well as incorporation of the C terminal residues of the neighboring catalytic monomer to create the ion pocket. The reasons behind this appear to be the lack of the IMP C2 and N3 in the RMP inhibitor, which cause the hydrophobic Ile318, which

normally forms hydrophobic contacts with the purine ring of the substrate or product, to move away from the more polar, less hydrophobic purine derivative. More importantly, with this portion of the purine ring absent, it is now more favorable for the active site cysteine (Cys319) to move into its catalytic position without the need for the NAD⁺ cofactor to bind and for catalysis to occur. This would not be the case with substrate or product present as the Cys319 sulfhydryl would be within 2.8 of the C2 position of IMP or within 1.5 of the oxygen bound to the C2 position of XMP.

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It appears that in mammalian IMPDH and the presented T. foetus structures, the covalent intermdiate is necessary to recruit the ion to the active site whereas the inhibitor ribavirin allows the active site loop to occupy this position without forming a covalent bond with the enzyme. No ion was found in our T. foetus IMP bound structure. In the human IMPDH structure with the covalently bound inhibitor 6-Cl IMP, no cation was present because it was necessary for the active site loop to move from the purine ring C2 position to the inhibitor C6 position in order for the active site cysteine to form a covalent bond with the inhibitor. This movement in the loop prevented formation of the ion-binding pocket. Furthermore, the acitve site loop in the apo S. pyogenes structure is in this cation-binding conformation without a covalent intermediate and a possible ion, designated water 179 (PDB accession code IZFJ), appears to occupy the same cation position as in the Chinese hamster (PDB accession code 1JR1) and the T. foetus structures presented here. The IMP in the bacterial structure is

not covalently bound and the C2 of the purine ring is rotated slightly away from the active site cysteine. In the *T. foetus* IMP structure, it is the loop that moves slightly away from C2 of IMP when compared to the hamster covalently bound structure and the *B. burgdorferi* apostructure.

The bacterial acitve site loop appears to be stabilized upon substrate binding by Thr310, which also makes hydrogen bonds with the active site flap, both directly and through an ordered water. This threonine is conserved in bacteria but is substituted with an isoleucine in eukaryotes, which appears to disrupt the structural coupling of the active site loop to the active This results in a partial destabilization of site flap. the active site loop allowing the active site cysteine to be displaced instead of the substrate. The bacterial acitve site loop is in the catalytic position immediately following substrate binding, and this could explain the ten fold higher Kcat compared to the mammalian and T. foetus enzymes (24, 2, 1.8 and 4 s-1 for S. pyogenes, T. foetus, and human type I and II, respectively) (Digits and Hedstrom, supra, (1999); Zhang et al., supra, (1999); Hager et al., Biochem. Pharmacol. 49:1323-1329 (1995)).

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The mammalian and *T. foetus* enzymes, at some point after substrate binding, must first move the active site loop into position; recruit the active site cation and C-terminal residues of the neighboring monomer before catalysis is possible. These steps may be coupled to cofactor binding. If the positively charged NAD⁺ binds over the C2 position of IMP it may expose the substrate

C2 to the active site cysteine thiol for subsequent nucleophilic attack. A role for the active site ion may be in stabilization of the active site loop during catalysis. The carbonyl oxygen from the active site Cys319 forms part of the cation binding site. When this site is occupied, the cysteine is in an ideal position to form a covalent bond with the C2 carbon of IMP. The cation-binding site appears to be formed before covalent bonding in bacterial IMPDH but likely occurs during covalent bond formation in mammalian and T. foetus IMPDH.

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In the steady-state kinetic analysis of T. foetus IMPDH, an apparent Km of 3.0 μM for IMP was observed. This is consistent with the previously published Km value of 1.7 μM from a detailed bisubstrate kinetic analysis (Digits and Hedstrom, supra, (1999)). This value is much smaller than the Km of 14.2 and 9.2 μM , respectively, for human type I and II IMPDH (Hager et al., supra, (1995)) as well as the Km of 62 μM for S. pyogenes enzyme (Zhang et al., supra, (1999)). 20 result indicates the IMP binds to T. foetus IMPDH about 3 to 5-fold tighter than to mammalian enzymes. Interestingly, RMP, a nucleotide inhibitor, was shown to This is about 5 have a Ki of 65 nM for T. foetus IMPDH. to 10-fold lower than the Ki for human type I and II 25 IMPDH, where the values are 650 nM and 390 nM, respectively (Hager et al., supra, (1995)). And it is considerably lower than the Ki of 6 μM for S. pyogenes IMPDH (Zhang et al., supra, (1999)). This result is consistent with steady-state kinetic analysis that shows 30 that T. foetus IMPDH binds IMP (or the IMP analog RMP)

more tightly than IMPDH from other species. Furthermore, the inhibition studies with RMP demonstrated that specifies specificity for an inhibitor does not occur in IMPDH. Our in vitro studies showed that RMP is a potent nanomolar inhibitor for *T. foetus* IMPDH and it appears that RMP is more effective against the protist form of IMPDH than the human and bacterial forms. A structural explanation for the 100 fold difference in Ki between *T. foetus* and *S. pyogenes* IMPDH could not be established from the highly conserved substrate binding site. The differences in Ki may be related, at least in part, to the kinetic mechanism. Further in vivo experiments are needed to address whether there is any clinical significance and pharmacological effects of ribavirin on *T. foetus*-infected cows.

Methods for expression, purification, and crystallization of *T. foetus* IMPDH.

Recombinant *T. foetus* IMPDH enzyme was produced from a pBAce plasmid (Chin and Wang, supra, (1994)) containing the gene for *T. foetus* IMPDH (Beck et al., Exp. Parasitol. 78:101-112 (1994)) that was transformed into Escherichia coli strain H712 (E. coli Stock Center, Yale University, New Haven, CT). Expression of *T. foetus* IMPDH was achieved by modifying previously published protocols (Craig et al., Proc. Natl. Acad. Sci. USA 88:2500-2504 (1991); Neidhardt et al., J. Bacteriol. 119:736-747 (1974); Yuan et al., J. Biol. Chem. 265:13528-13532(1990)). Briefly, the cells were grown in MOPS media in a 19-liter fermentor (Wheaton Science

Products, Millville, NJ.) and were inoculated with 0.5 liters of overnight MOPS culture of H712 containing the IMPDH plasmid. The fermentation was kept at 37° C and was maintained by aeration, stirring and glucose addition. The dissolved oxygen (DO) was maintained at greater than 40%. The cells were harvested at 8 hours when the DO dropped to below 20% at an OD₆₀₀ of roughly 1.5.

The cells were concentrated to 0.5 L by tangential flow filtration (Millipore, Inc., Bedford, Ma.) and pelleted by centrifugation at 6,000 g. pellet was re-suspended in a three fold volume of buffer A (50 mM Tris pH 8, 50 mM KCl, 10% gycerol, and 1 mM 2mercaptoethanol) supplemented with protease inhibitors and 1mM EDTA, and was then flash frozen in liquid nitrogen before storage at -85°C. This mixture was lysed by French Press and the lysate was clarified by centrifugation at 20,000 g. The supernatant was then run over a cibacron blue column on an AKTA FPLC (Amersham-Pharmacia). Protein was eluted from the column with 1 M This was followed by dialysis into buffer A and concentration to 15 mg/ml. The protein was then passed through a monoQ column (Amersham-Pharmacia) using a gradient from 50 to 500 mM KCl over 20 column volumes. The resulting protein was >90% pure and was dialyzed in 25 buffer A and concentrated to 30 mg/ml for storage at -85°C.

The protein was crystallized at 20°C by mixing

15 mg/ml protein in buffer A into 42% of saturated sodium malonate, 100 mM Tris pH 8.0, 4 mM PEG 400, and 1 mM 2-

mercaptoethanol in 6µl sitting drops in a 1:1 ration of well solution to protein. The protein was also cocrystallized with a ten-fold molar excess of RMP. For the efforts to co-crystallize both RMP and MOA with IMPDH, saturating levels of MOA were added to newly formed RMP bound crystals. These crystals were allowed to soak for several hours to several days before cryomounting.

10 Throughout this application various publications have been referenced within parentheses. The disclosures of these publications in their entireties are hereby incorporated by reference in this application in order to more fully describe the state of the art to which this invention pertains.

Although the invention has been described with reference to the disclosed embodiments, those skilled in the art will readily appreciate that the specific experiments detailed are only illustrative of the invention. It should be understood that various modifications can be made without departing from the spirit of the invention.

TABLE 1. Data collection and refinement statistics.

Structure	IMP	IMP+MPA	XMP+MPA	NAD+XMP
Wavelength (Å)	0.97	0.97	0.97	1.00
Resolution Range (Å)	50 - 2.2	50 - 1.95	50 - 2.2	20 - 2.15
Resolution of outer shell (Å)	2.2-2.34	1.95-2.07	2.2-2.34	2.15-2.28
R (R _{free}) (%)	24.9 (27.1)	24.0 (26.8)	22.5 (25.6)	22.3 (24.6)
Unique reflections	32,418	45,540	32,987	33,857
Total observations	996,397	1,036,471	407,857	734,853
I/o _l all/outer shell	21.7/2.13	25.88/1.82	21.38/2.88	19.03/2.22
R _{sym} all/outer shell (%)	6.4/59.6	5.7/66.8	6.6/53.8	8.0/57.8
Completeness all/outer shell	99.9/99.8	99.0/95.7	99.5/98.7	98.4/95.9
(%)			. "	
Degrees collected	37.5	37.5	20	30
Amino acid residues in model	2-101, 222-	2-106, 222-	2-101, 222-	2-101, 222-
	416, 431-483	416, 430-483	417, 428-483	317, 322-416,
				428-483
Number of water molecules	159	202	183	172
Cell dimensions	154.4	153.5	155.1	153.8
a=b=c (Å)				·· .
Bond length dev. (Å)	0.006	0.006	0.005	0.007
Bond angle dev. (°)	1.2	1.2	1.1	1.3
Dihedral angle dev. (°)	22.9	22.2	22.5	23.0
Improper angle dev. (°)	0.71	0.70	0.67	0.80
Ramachandran	91.9/7.8/0.3	92.1/7.9/0.0	90.7/9.0/0.3	91.7/7.9/0.3
core/allowed/			•	
generously allowed (%)				
Mosaicity (°)	0.60	0.65	0.40	0.70

```
08-AUG-02
                                                          1ME9
HEADER OXIDOREDUCTASE
TITLE
        INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
       2 TRITRICHOMONAS FOETUS WITH IMP BOUND
TITLE
COMPND 2 MOLECULE: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE;
COMPND 3 CHAIN: A;
COMPND 4 SYNONYM: IMP DEHYDROGENASE, IMPDH;
COMPND 5 EC: 1.1.1.205;
COMPND 6 ENGINEERED: YES
SOURCE MOL ID: 1;
SOURCE 2 ORGANISM SCIENTIFIC: TRITRICHOMONAS FOETUS;
SOURCE 3 GENE: IMPDH;
SOURCE 4 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE 5 EXPRESSION SYSTEM COMMON: BACTERIA;
SOURCE 6 EXPRESSION SYSTEM STRAIN: H712;
SOURCE 7 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE 8 EXPRESSION_SYSTEM_PLASMID: PBACE
KEYWDS ALPHA BETA BARREL
EXPDTA X-RAY DIFFRACTION
AUTHOR G. L. PROSISE, H. LUECKE
         AUTH G. L.PROSISE, H.LUECKE
JRNL
          TITL CRYSTAL STRUCTURE OF T. FOETUS INOSINE
JRNL
         TITL 2 MONOPHOSPHATE DEHYDROGENASE IN COMPLEX WITH
JRNL
        TITL 3 SUBSTRATE, COFACTOR, AND ANALOGS:STRUCTURAL BASIS TITL 4 FOR THE RANDOM-IN ORDERED-OUT KINETIC MECHANISM
JRNL
JRNL
JRNL
         REF
                 TO BE PUBLISHED
JRNL
         REFN
REMARK 1
REMARK 2
REMARK 2 RESOLUTION. 2.20 ANGSTROMS.
REMARK 3
REMARK 3 REFINEMENT.
REMARK 3 PROGRAM : CNS 1.1
REMARK 3 AUTHORS
                      : BRUNGER, ADAMS, CLORE, DELANO, GROS, GROSSE-
REMARK 3
                       : KUNSTLEVE, JIANG, KUSZEWSKI, NILGES, PANNU,
REMARK 3
                       : READ, RICE, SIMONSON, WARREN
REMARK 3
REMARK 3 REFINEMENT TARGET : ENGH & HUBER
REMARK 3
REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.20
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS): 19.77
REMARK 3 DATA CUTOFF
                                  (SIGMA(F)) : 0.000
REMARK 3 OUTLIER CUTOFF HIGH (RMS(ABS(F))) : NULL
REMARK 3 COMPLETENESS (WORKING+TEST) (%): 99.8
REMARK 3
          NUMBER OF REFLECTIONS
                                            : 32418
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
        3 CROSS-VALIDATION METHOD
REMARK
                                           : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING SET): 0.248
REMARK 3 FREE R VALUE
                                           : 0.273
REMARK 3 FREE R VALUE TEST SET SIZE (%): 5.200
REMARK
        3 FREE R VALUE TEST SET COUNT
REMARK 3 ESTIMATED ERROR OF FREE R VALUE : 0.007
REMARK 3
```

REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.

55

```
REMARK 3 TOTAL NUMBER OF BINS USED
                                      (A) : 2.20
          BIN RESOLUTION RANGE HIGH
REMARK 3
REMARK 3 BIN RESOLUTION RANGE LOW (A): 2.34
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%): 99.80
REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 5035
REMARK 3 BIN R VALUE
                              (WORKING SET): 0.2770
REMARK 3 BIN FREE R VALUE
                                       : 0.3040
REMARK 3 BIN FREE R VALUE TEST SET SIZE (%): 4.90
REMARK 3 BIN FREE R VALUE TEST SET COUNT : 262
REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.019
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS
                          : 2685
REMARK 3 NUCLEIC ACID ATOMS
                                 : 0
REMARK 3 HETEROGEN ATOMS
                                 : 24
REMARK 3
REMARK 3
          SOLVENT ATOMS
                                 : 145
REMARK 3 B VALUES.
                             (A**2) : 28.10
REMARK 3 FROM WILSON PLOT
REMARK 3 MEAN B VALUE (OVERALL, A**2): 40.20
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : 0.00000
REMARK 3 B22 (A**2) : 0.00000
REMARK 3 B33 (A**2) : 0.00000
REMARK 3 B12 (A**2) : 0.00000
REMARK 3 B13 (A**2) : 0.00000
REMARK 3 B23 (A**2) : 0.00000
REMARK 3
REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM LUZZATI PLOT
                                     (A) : 0.30
REMARK 3 ESD FROM SIGMAA
                                     (A) : 0.22
REMARK 3
          LOW RESOLUTION CUTOFF
                                     (A): 5.00
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT (A): 0.34
REMARK 3 ESD FROM C-V SIGMAA
                                     (A) : 0.25
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK
        3 BOND LENGTHS
3 BOND ANGLES (DEGR
                                     (A) : 0.006
REMARK 3 DIHEDRAL ANGLES (DEGREES): 1.20
REMARK 3 IMPROPER ANGLES (DEGREES): 22.80
REMARK 3 IMPROPER ANGLES (DEGREES): 0.70
REMARK 3
REMARK 3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                             RMS SIGMA
REMARK
        3
          MAIN-CHAIN BOND (A**2): 1.270; 1.500
          MAIN-CHAIN ANGLE
REMARK 3
                                     (A**2) : 2.150 ; 2.000
                                     (A**2) : 1.930 ; 2.000
REMARK 3 SIDE-CHAIN BOND
REMARK 3 SIDE-CHAIN ANGLE
                                     (A**2) : 2.840 ; 2.500
REMARK 3
REMARK 3 BULK SOLVENT MODELING.
REMARK 3 METHOD USED : FLAT MODEL
REMARK 3 KSOL : 0.36
REMARK 3 BSOL
                     : 40.24
REMARK
REMARK 3 NCS MODEL : NULL
```

```
REMARK
                                                        SIGMA/WEIGHT
REMARK 3 NCS RESTRAINTS.
                                                   RMS
REMARK 3 NCS RESTRAINTS.

REMARK 3 GROUP 1 POSITIONAL (A): NULL; NULL

REMARK 3 GROUP 1 B-FACTOR (A**2): NULL; NULL
REMARK 3
REMARK 3 PARAMETER FILE 1 : PROTEIN REP.PARAM
REMARK 3 PARAMETER FILE 2 : PARAM.GNSOL
REMARK 3 PARAMETER FILE 3 : CIS_PEPTIDE.PARAM
REMARK 3 PARAMETER FILE 4 : IMP.PAR
REMARK 3 PARAMETER FILE 5 : ION.PARAM
REMARK 3 PARAMETER FILE 6 : NULL
REMARK 3 TOPOLOGY FILE 1 : PROTEIN.TOP
REMARK 3 TOPOLOGY FILE 2 : IMP.TOP
REMARK 3 TOPOLOGY FILE 3 : MPA.TOP
REMARK 3 TOPOLOGY FILE 4
                             : ION.TOP
REMARK 3 TOPOLOGY FILE 5 : TOPH.GNSOL
REMARK 3 TOPOLOGY FILE 6 : NULL
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: NULL
REMARK 4
REMARK 4 1ME9 COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 09-AUG-2002.
REMARK 100 THE RCSB ID CODE IS RCSB016851.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION REMARK 200 DATE OF DATA COLLECTION : 11-APR-2001
REMARK 200 TEMPERATURE (KELVIN) : 100.0
                                       .: 7.50
REMARK 200 PH
REMARK 200 NUMBER OF CRYSTALS USED
REMARK 200
REMARK 200 SYNCHROTRON (Y/N) : Y
REMARK 200 RADIATION SOURCE : SSRL
REMARK 200 BEAMLINE
                                     : NULL
REMARK 200 X-RAY GENERATOR MODEL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A): 0.97
REMARK 200 MONOCHROMATOR
                                          : NULL
                                          : NULL
REMARK 200 OPTICS
REMARK 200
REMARK 200 DETECTOR TYPE
                                         : IMAGE PLATE
REMARK 200 DETECTOR MANUFACTURER
                                         : MARRESEARCH
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE : SCALEPACK
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 32513
REMARK 200 RESOLUTION RANGE HIGH (A): 2.200
REMARK 200 RESOLUTION RANGE LOW (A): 20.000
REMARK 200 REJECTION CRITERIA (SIGMA(I)): 0.000
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE (%): 99.9
                                        : 6.700
REMARK 200 DATA REDUNDANCY
REMARK 200 R MERGE
                                      (I) : 0.06400
REMARK 200 R SYM
                                      (I) : NULL
REMARK 200 <I/SIGMA(I) > FOR THE DATA SET : 21.7000
```

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REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.20
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.24
REMARK 200 COMPLETENESS FOR SHELL (%): 99.8
REMARK 200 DATA REDUNDANCY IN SHELL : NULL
REMARK 200 R SYM FOR SHELL
REMARK 200 STATESTA
                                           (I) : 0.59600
                                         (I) : NULL
REMARK 200 <I/SIGMA(I) > FOR SHELL
                                              : 2.130
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: FOURIER SYNTHESIS
REMARK 200 SOFTWARE USED: CNS
REMARK 200 STARTING MODEL: PDB ENTRY 1AK5
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: SODIUM MALONATE, TRIS, 2-
REMARK 280 MERCAPTOETHANOL, EDTA, GLYCEROL
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 4 3 2
REMARK 290
REMARK 290
                 SYMOP SYMMETRY
REMARK 290
               NNNMMM OPERATOR
REMARK 290
                 1555
                         X,Y,Z
REMARK 290 2555 -X,-Y,Z
REMARK 290 3555 -X,Y,-Z
REMARK 290 4555 X,-Y,-Z
REMARK 290 4555 X,-1,-2
REMARK 290 5555 Z,X,Y
REMARK 290 6555 Z,-X,-Y
REMARK 290 7555 -Z,-X,-Y
REMARK 290 8555 -Z,X,-Y
REMARK 290 9555 Y,Z,X
REMARK 290 10555 -Y,Z,-X
REMARK 290 11555 Y,-Z,-X
REMARK 290 12555 -Y,-Z,X
REMARK 290 13555 Y,X,-Z
               14555 -Y,-X,-Z
REMARK 290
REMARK 290
                15555 Y,-X,Z
REMARK 290
                16555 -Y,X,Z
REMARK 290
                 17555 X,Z,-Y
                18555
REMARK 290
                          -X,Z,Y
                19555
REMARK 290
                          -X,-Z,-Y
REMARK 290
                20555 X,-Z,Y
REMARK 290
                21555 Z,Y,-X
               22555 Z,-Y,X
23555 -Z,Y,X
24555 -Z,-Y,-
REMARK 290
REMARK 290
REMARK 290
                          -Z,-Y,-X
REMARK 290
REMARK 290 WHERE NNN -> OPERATOR NUMBER
               MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290
```

REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY REMARK 290 RELATED MOLECULES. 1 1.000000 0.000000 0.000000 1 0.000000 1.000000 0.000000 REMARK 290 SMTRY1 0.00000 REMARK 290 SMTRY2 0.00000 REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 3 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 3 0.000000 1.000000 0.000000 0.00000 SMTRY3 3 0.000000 0.000000 -1.000000 REMARK 290 0.00000 REMARK 290 SMTRY1 4 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 4 0.000000 -1.000000 0.000000 0.00000 SMTRY3 4 0.000000 0.000000 -1.000000 REMARK 290 0.00000 5 0.000000 0.000000 1.000000 5 1.000000 0.000000 0.000000 SMTRY1 0.00000 REMARK 290 REMARK 290 SMTRY2 0.00000 REMARK 290 SMTRY3 5 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY1 6 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY2 6 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 6 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY1 7 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY2 7 -1.000000 0.000000 0.000000 0.00000 SMTRY3 7 0.000000 1.000000 0.000000 REMARK 290 0.00000 SMTRY1 8 0.000000 0.000000 -1.000000 REMARK 290 0.00000 REMARK 290 SMTRY2 8 1.000000 0.000000 0.000000 SMTRY3 8 0.000000 -1.000000 0.000000 0.00000 REMARK 290 0.00000 SMTRY1 9 0.000000 1.000000 0.000000 SMTRY2 9 0.000000 0.000000 1.000000 REMARK 290 0.00000 SMTRY2 9 0.000000 0.000000 1.000000 SMTRY3 9 1.000000 0.000000 0.000000 REMARK 290 0.00000 REMARK 290 0.00000 SMTRY1 10 0.000000 -1.000000 0.000000 REMARK 290 0.00000 REMARK 290 SMTRY2 10 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY3 10 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 11 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 11 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY3 11 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 12 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 12 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY3 12 1.000000 0.000000 0.000000 0.00000 SMTRY1 13 0.000000 1.000000 0.000000 REMARK 290 0.00000 REMARK 290 SMTRY2 13 1.000000 0.000000 0.000000 REMARK 290 SMTRY3 13 0.000000 0.000000 -1.000000 REMARK 290 SMTRY1 14 0.000000 -1.000000 0.000000 0.00000 0.00000 0.00000 REMARK 290 SMTRY2 14 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 14 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY1 15 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 15 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 15 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 16 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 16 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 16 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 17 1.000000 0.000000 0.000000 0.00000 SMTRY2 17 0.000000 0.000000 1.000000 REMARK 290 0.00000 SMTRY3 17 0.000000 -1.000000 0.000000 REMARK 290 0.00000 SMTRY1 18 -1.000000 0.000000 0.000000 REMARK 290 0.00000 REMARK 290 SMTRY2 18 0.000000 0.000000 1.000000 0.00000

```
REMARK 290 SMTRY3 18 0.000000 1.000000 0.000000
                                                     0.00000
REMARK 290 SMTRY1 19 -1.000000 0.000000 0.000000
                                                    0.00000
REMARK 290 SMTRY2 19 0.000000 0.000000 -1.000000
                                                    0.00000
REMARK 290 SMTRY3 19 0.000000 -1.000000 0.000000
                                                    0.00000
REMARK 290 SMTRY1 20 1.000000 0.000000 0.000000
                                                     0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 1 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.00000
                                                   0.00000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000
0.00000
REMARK 350 BIOMT2 4 1.000000 0.000000 0.000000
REMARK 350 BIOMT3 4 0.000000 0.000000 1.000000
                                                    0.00000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465
          M RES C SSSEQI
          MET A 1
REMARK 465
REMARK 465
            GLY A
                    102
```

REMARK	465	PHE A	103
REMARK	465	VAL A	104
REMARK	465	VAL A	105
REMARK	465	SER A	106
REMARK	465	ASP A	107
REMARK	465	SER A	108
REMARK	465	ASN A	109
REMARK	465	VAL A	110
REMARK	465	LYS A	111
REMARK	465	PRO A	112
REMARK	465	ASP A	113
REMARK	465	GLN A	114
REMARK	465	THR A	115
REMARK	465	PHE A	116
REMARK	465	ALA A	117
REMARK	465	ASP A	118
REMARK	465	VAL A	119
REMARK	465	LEU A	120
REMARK	465	ALA A	121
REMARK	465	ILE A	122
REMARK	465	SER A	123
REMARK	465	GLN A	124
REMARK	465	ARG A	125
REMARK	465	THR A	126
REMARK	465	THR A	127
REMARK	465	HIS A	128
REMARK	465	ASN A	129
REMARK	465	THR A	130
REMARK	465	VAL A	131
REMARK	465	ALA A	132
REMARK	465	VAL A	133
REMARK	465	THR A	134
REMARK	465	ASP A	135
REMARK	465	ASP A	136
REMARK	465	GLY A	137
REMARK	465	THR A	138
REMARK	465	PRO A	139
REMARK	465	HIS A	140
REMARK	465	GLY A	141
REMARK	465	VAL A	142
REMARK	465	LEU A	143
REMARK	465	LEU A	144
REMARK		GLY A	145
REMARK	465	LEU A	146
REMARK	465	VAL A	147
REMARK	465	THR A	148
REMARK	465	GLN A	149
REMARK	465	ARG A	150
REMARK	465	ASP A	151
REMARK	465	TYR A	152
REMARK	465	PRO A	153
REMARK	465	ILE A	154
REMARK	465	ASP A	155
REMARK	465	LEU A	156
REMARK	465	THR A	157
REMARK	465	GLN A	158
REMARK	465	THR A	159
VINITALIVITY.	-UJ	THIK M	109

REMARK	465	GLU	Α	160
REMARK	465	THR	A	161
REMARK	465	LYS	A	162
REMARK	465	VAL	Α	163
REMARK	465	SER	Α	164
REMARK	465	ASP	Α	165
REMARK	465	MET	Α	166
REMARK	465	MET	A	167
REMARK	465	THR	A	168
REMARK	465	PRO	A	169
REMARK	465	PHE	A	170
REMARK	465	SER	A	171
REMARK	465	LYS	A	172
REMARK	465	LEU	A	173
REMARK	465	VAL	A	174
	465			175
REMARK		THR	A	
REMARK	465	ALA		176
REMARK	465	HIS		177
REMARK	465	GLN		178
REMARK		ASP	A	179
REMARK	465	THR	A	180
REMARK	465	LYS	A	181
REMARK	465	LEU	Α	182
REMARK	465	SER	Α	183
REMARK	465	GLU	A	184
REMARK	465	ALA	Α	185
REMARK	465	ASN	Α	186
REMARK	465	LYS	Α	187
REMARK	465	ILE	Α	188
REMARK	465	ILE	Α	189
REMARK	465	TRP	Α	190
REMARK	465	GLU		191
REMARK	465	LYS		192
REMARK		LYS		193
REMARK	465	LEU		194
REMARK	465	ASN		195
REMARK	465	ALA		196
REMARK	465	LEU		197
REMARK		PRO		198
REMARK		ILE		199
REMARK		ILE		200
REMARK				201
		ASP		
REMARK		ASP		202
REMARK	465	ASP		203
REMARK	465	GLN		204
REMARK	465	HIS		205
REMARK	465	LEU		206
REMARK		ARG		207
REMARK		TYR		208
REMARK		ILE		209
REMARK		VAL		210
REMARK	465	PHE		211
REMARK	465	ARG	A	212
REMARK	465	LYS	A	213
REMARK	465	ASP	A	214
REMARK	465	TYR	A	215
REMARK	465	ASP	A	216

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REMARK 465
            ARG A
            SER A 218
REMARK 465
            GLN A
                   219
REMARK 465
            VAL A
                     220
REMARK 465
            CYS A
                     221
REMARK 465
            GLN A
                    417
REMARK 465
            ARG A
                    418
REMARK 465
            TYR A 419
REMARK 465
            ASP A 420
REMARK 465
            LEU A 421
REMARK 465
            GLY A 422
REMARK 465
             GLY A 423
REMARK 465
                    424
             LYS A
REMARK 465
             GLN A
REMARK 465
            LYS A 426
REMARK 465
            LEU A 427
REMARK 465
            SER A 428
REMARK 465
REMARK 465
            VAL A 484
            GLU A 485
GLY A 486
GLY A 487
REMARK 465
REMARK 465
REMARK 465
           ALA A
REMARK 465
                     488
            HIS A 489
ASP A 490
REMARK 465
REMARK 465
            VAL A 491
REMARK 465
            ILE A 492
REMARK 465
REMARK 465
            VAL A 493
REMARK 465
            LYS A 494
            ASP A 495
REMARK 465
            ARG A 496
ILE A 497
ASN A 498
REMARK 465
REMARK 465
REMARK 465
REMARK 465 ASP A · 499
            TYR A 500
REMARK 465
REMARK 465
            HIS A 501
             PRO A
                      502
REMARK 465
REMARK 465
              LYS A
                      503
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS
REMARK 500
REMARK 500 THE FOLLOWING ATOMS THAT ARE RELATED BY CRYSTALLOGRAPHIC
REMARK 500 SYMMETRY ARE IN CLOSE CONTACT. AN ATOM LOCATED WITHIN 0.15
REMARK 500 ANGSTROMS OF A SYMMETRY RELATED ATOM IS ASSUMED TO BE ON A
REMARK 500 SPECIAL POSITION AND IS, THEREFORE, LISTED IN REMARK 375
REMARK 500 INSTEAD OF REMARK 500. ATOMS WITH NON-BLANK ALTERNATE
REMARK 500 LOCATION INDICATORS ARE NOT INCLUDED IN THE CALCULATIONS.
REMARK 500
REMARK 500 DISTANCE CUTOFF:
REMARK 500 2.2 ANGSTROMS FOR CONTACTS NOT INVOLVING HYDROGEN ATOMS
REMARK 500 1.6 ANGSTROMS FOR CONTACTS INVOLVING HYDROGEN ATOMS
REMARK 500
REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI SSYMOP DISTANCE
                                     K A 900 16655
                                                           2.18
                 GLY A 20
                               K
REMARK 500 O
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
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63

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REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1
                              ATM2
                                      EMTA
REMARK 500
           ILE A 27
                             - CA - C
                                          ANGL. DEV. = -8.1 DEGREES
                        N
REMARK 500
            SER A 63
                             - CA - C
                                          ANGL. DEV. = 7.9 DEGREES
                         N
             GLY A 305
                             - CA - C
                                          ANGL. DEV. = 7.8 DEGREES
REMARK 500
                         N
                             - CA - ι C
                                          ANGL. DEV. = 7.2 DEGREES
REMARK 500
             GLY A 312
                         N
                            - CA - C
REMARK 500
             SER A 357
                         N
                                           ANGL. DEV. = -7.4 DEGREES
                                           ANGL. DEV. = 8.0 DEGREES
REMARK 500
             LYS A 472
                        N
                                         ANGL. DEV. = -9.2 DEGREES
REMARK 500
           LYS A 474 N - CA - C
                       N - CA - C ANGL. DEV. = -7.8 DEGREES
REMARK 500
           LEU A 477
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1AK5
                             RELATED DB: PDB
REMARK 900 INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
REMARK 900 TRITRICHOMONAS FOETUS
REMARK 900 RELATED ID: 1ME7
                            RELATED DB: PDB
REMARK 900 1ME7 CONTAINS THE SAME PROTEIN WITH RMP AND MPA BOUND
REMARK 900 RELATED ID: 1ME8 RELATED DB: PDB
REMARK 900 1ME8 CONTAINS THE SAME PROTEIN WITH RMP BOUND
REMARK 900 RELATED ID: 1MEH RELATED DB: PDB
REMARK 900 1MEH CONTAINS THE SAME PROTEIN WITH IMP AND MPA BOUND
REMARK 900 RELATED ID: 1MEI RELATED DB: PDB
REMARK 900 1MEI CONTAINS THE SAME PROTEIN WITH XMP AND MYCOPHENOLIC
REMARK 900 ACID BOUND
REMARK 900 RELATED ID: 1MEW
                             RELATED DB: PDB
REMARK 900 1MEW CONTAINS THE SAME PROTEIN WITH XMP AND NAD BOUND
              1 503 SWS
                              P50097
                                        IMDH TRIFO
DBREF 1ME9 A
                                                      1
SEQADV 1ME9 CSO A 319 SWS P50097
                                     CYS 319 MODIFIED RESIDUE
       1 A 503 MET ALA LYS TYR TYR ASN GLU PRO CYS HIS THR PHE ASN
SEQRES
         2 A 503 GLU TYR LEU LEU ILE PRO GLY LEU SER THR VAL ASP CYS
SEQRES
        3 A 503 ILE PRO SER ASN VAL ASN LEU SER THR PRO LEU VAL LYS
SEQRES
        4 A 503 PHE GLN LYS GLY GLN GLN SER GLU ILE ASN LEU LYS ILE
SEORES
SEQRES
        5 A 503 PRO LEU VAL SER ALA ILE MET GLN SER VAL SER GLY GLU
       6 A 503 LYS MET ALA ILE ALA LEU ALA ARG GLU GLY GLY ILE SER
SEQRES
       7 A 503 PHE ILE PHE GLY SER GLN SER ILE GLU SER GLN ALA ALA
SEQRES
       8 A 503 MET VAL HIS ALA VAL LYS ASN PHE LYS ALA GLY PHE VAL
SEQRES
SEQRES
       9 A 503 VAL SER ASP SER ASN VAL LYS PRO ASP GLN THR PHE ALA
SEORES 10 A 503 ASP VAL LEU ALA ILE SER GLN ARG THR THR HIS ASN THR
SEORES 11 A 503 VAL ALA VAL THR ASP ASP GLY THR PRO HIS GLY VAL LEU
SEQRES 12 A 503 LEU GLY LEU VAL THR GLN ARG ASP TYR PRO ILE ASP LEU
SEQRES 13 A 503 THR GLN THR GLU THR LYS VAL SER ASP MET MET THR PRO
SEQRES 14 A 503 PHE SER LYS LEU VAL THR ALA HIS GLN ASP THR LYS LEU
SEQRES 15 A 503 SER GLU ALA ASN LYS ILE ILE TRP GLU LYS LYS LEU ASN SEQRES 16 A 503 ALA LEU PRO ILE ILE ASP ASP GLN HIS LEU ARG TYR
SEQRES 17 A 503 ILE VAL PHE ARG LYS ASP TYR ASP ARG SER GLN VAL CYS
SEQRES 18 A 503 HIS ASN GLU LEU VAL ASP SER GLN LYS ARG TYR LEU VAL
SEQRES 19 A 503 GLY ALA GLY ILE ASN THR ARG ASP PHE ARG GLU ARG VAL
```

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PRO ALA LEU VAL GLU ALA GLY ALA ASP VAL LEU CYS ILE
      20 A 503
SEORES
                 ASP SER SER ASP GLY PHE SER GLU TRP GLN LYS ILE THR
      21 A
            503
SEORES
                 ILE GLY TRP ILE ARG GLU LYS TYR GLY ASP LYS VAL LYS
SEORES 22 A 503
                 VAL GLY ALA GLY ASN ILE VAL ASP GLY GLU GLY PHE ARG
SEQRES 23 A 503
                 TYR LEU ALA ASP ALA GLY ALA ASP PHE ILE LYS ILE GLY
            503
SEQRES
       24 A
                  ILE GLY GLY GLY SER ILE CSO ILE THR ARG GLU GLN LYS
            503
SEORES 25 A
SEQRES 26 A 503 GLY ILE GLY ARG GLY GLN ALA THR ALA VAL ILE ASP VAL
SEQRES 27 A 503 VAL ALA GLU ARG ASN LYS TYR PHE GLU GLU THR GLY ILE
SEQRES 28 A 503 TYR ILE PRO VAL CYS SER ASP GLY GLY ILE VAL TYR ASP
SEORES 29 A 503 TYR HIS MET THR LEU ALA LEU ALA MET GLY ALA ASP PHE
SEQRES 30 A 503 ILE MET LEU GLY ARG TYR PHE ALA ARG PHE GLU GLU SER
SEQRES 31 A 503 PRO THR ARG LYS VAL THR ILE ASN GLY SER VAL MET LYS
SEQRES 32 A 503 GLU TYR TRP GLY GLU GLY SER SER ARG ALA ARG ASN TRP
SEQRES 33 A 503 GLN ARG TYR ASP LEU GLY GLY LYS GLN LYS LEU SER PHE
SEQRES 34 A 503 GLU GLU GLY VAL ASP SER TYR VAL PRO TYR ALA GLY LYS
SEQRES 35 A 503 LEU LYS ASP ASN VAL GLU ALA SER LEU ASN LYS VAL LYS
SEORES 36 A 503 SER THR MET CYS ASN CYS GLY ALA LEU THR ILE PRO GLN
SEQRES 37 A 503 LEU GLN SER LYS ALA LYS ILE THR LEU VAL SER SER VAL
SEQRES 38 A 503 SER ILE VAL GLU GLY GLY ALA HIS ASP VAL ILE VAL LYS
       39 A 503 ASP ARG ILE ASN ASP TYR HIS PRO LYS
SEQRES
MODRES 1ME9 CSO A 319 CYS S-HYDROXYCYSTEINE
      CSO A 319
                       7
HET
        K A 900
                      1
HET
                      23
      IMP 602
          CSO S-HYDROXYCYSTEINE
HETNAM
           K POTASSIUM ION
HETNAM
          IMP INOSINIC ACID
HETNAM
       1 CSO
                C3 H7 N1 O3 S1
FORMUL
                  K1 1+
FORMUL
       2
            K
        3 IMP
                 C10 H13 N4 O8 P1
FORMUL
        4 HOH
                *145(H2 O1)
FORMUL
                                                                        3
                                     5
                     11 ASN A
                                 13
           1 THR A
HELIX
        1
                                                                        5
                      27 VAL A
                                 31 5
           2 ILE A
HELIX
        2
                                                                       11
                                  74 1
            3 GLY A
                      64 GLU A
HELIX
         3
                                                                       14
                     85 ASN A
                                  98
                                     1
            4 SER A
HELIX
         4
                                                                       13
                     242
                         GLY A 254
                                     1
         5
            5 ASP A
HELIX
                                                                       16
                     267
                         GLY A
                                282
                                     1
         6
            6 SER A
HELIX
                                                                        3
                                 285
                                     5
            7 ASP A 283
                         VAL A
         7
HELIX
                                                                       11
            8 ASP A 294 ALA A 304 1
HELIX
        8
                                                                       21
                         GLY A 350 1
            9 GLY A 330
HELIX
        9
                                                                       11
           10 TYR A 363 MET A 373 1
HELIX
        10
                                                                        6
           11 GLY A 381 ARG A 386 1
HELIX
        11
                                                                        6
           12 SER A 410 ASN A 415 1
HELIX
        12
                                                                       20
            13 LYS A 442
                         CYS A 461
        13
                                     1
HELIX
        14
           14 THR A 465 ALA A 473
                                     1
HELIX
            A 2 TYR A 15 LEU A 17
                                     0
        1
SHEET
                                                       N LEU A 16
            A 2 ILE A 475
                          LEU A 477 -1
                                        O THR A 476
SHEET
         2
                           PRO A 36
                                     0
             B 2 THR A 35
SHEET
         1
                                                         THR A
                                                                35
             B 2 ASN A 49
                           LEU A 50 -1 O LEU A 50
                                                       N
SHEET
         2
             C 2 PHE A 40
                           GLN A 41
                                     0
SHEET
         1
                                                          PHE A
                                                                40
             C 2 ILE A 351
                           TYR A 352 -1
                                        O TYR A 352
                                                       N
SHEET
         2
       . 1
                           SER A 56
                                     0
             D 9 LEU A 54
SHEET
                                                       N SER A 56
             D 9 ILE A
                       77
                           ILE A 80
                                      1
                                        O ILE A 77
         2
SHEET
                                                       N ILE A 80
             D 9 GLY A 235
                           ILE A 238
                                      1
                                        0
                                           GLY A 237
         3
SHEET
                                        0
                                           CYS A 259
                                                       N ILE A 238
             D 9 VAL A 257
                           ILE A 260
                                      1
SHEET
                                                       N LEU A 258
                                      1 O GLY A 288
             D 9 VAL A 287 ILE A 292
SHEET
             D 9 PHE A 308 ILE A 311 1 O LYS A 310
                                                       N ALA A 289
 SHEET
```

9

65

```
D 9 VAL A 355
                              ASP A 358
                                                 CYS A 356
                                                                  ILE A 311
SHEET
         7
                                          1
                                              0
SHEET
              D 9 PHE A 377
                              LEU A 380
                                          1
                                              0
                                                 MET A 379
                                                              N
                                                                  SER A 357
         8
                                     56
                                                 VAL A 55
                                                                  ILE A 378
              D 9 LEU A
                              SER A
                                          1
                                              Ν
                                                              0
SHEET
         9
                         54
SHEET
         1
              E 3 LYS A 394
                              ILE A 397
                                           0
              E 3 SER A 400
                              TRP A 406 -1
                                              0
                                                 SER A 400
                                                              Ν
                                                                  ILE A 397
SHEET
                              PRO A 438 ~1
                                                                  TYR A 405
SHEET
              E 3 ASP A 434
                                              0
                                                 SER A 435
SSBOND
         1 CYS A
                    26
                           CYS A 459
CISPEP
         1 GLY A
                           ASN A 291
                                                 0 .
                                                            0.99
                  290
        154.412 154.412 154.412 90.00
                                              90.00 90.00 P 4 3 2
CRYST1
                                                                           24
ORIGX1
             1.000000
                       0.000000 0.000000
                                                     0.00000
ORIGX2
             0.000000
                       1.000000
                                  0.000000
                                                     0.00000
ORIGX3
             0.000000
                       0.000000
                                   1.000000
                                                     0.00000
                       0.000000
SCALE1
             0.006476
                                   0.000000
                                                     0.00000
SCALE2
             0.000000
                       0.006476
                                   0.000000
                                                     0.00000
                       0.000000
SCALE3
             0.000000
                                   0.006476
                                                     0.00000
MOTA
           1
             N
                  ALA A
                           2
                                   55.031
                                           74.792
                                                     36.719
                                                             1.00 34.77
                                                                                    Ν
MOTA
           2
              CA
                  ALA A
                           2
                                   55.778
                                            73.707
                                                     36.025
                                                             1.00 35.14
                                                                                     C
MOTA
           3
              С
                  ALA A
                                            73.393
                                                     36.732
                                                             1.00 35.76
                                                                                     C
                           2
                                   57.099
                                                             1.00 33.95
                                                                                     0
MOTA
           4
              0
                  ALA A
                           2
                                   57.541
                                            74.137
                                                     37.609
                                                                                     С
MOTA
           5
              CB
                  ALA A
                           2
                                   56.041
                                            74.107
                                                     34.583
                                                             1.00 34.68
MOTA
           6
              N
                  LYS A
                           3
                                   57.724
                                            72.288
                                                     36.340
                                                             1.00 35.35
                                                                                    N
MOTA
           7
              CA
                  LYS A
                           3
                                   58.992
                                            71.873
                                                     36.927
                                                             1.00 37.15
                                                                                     C
                                                                                     C
MOTA
           8
              C
                  LYS A
                           3
                                   60.102
                                            72.070
                                                     35.899
                                                             1.00 36.78
           9
                                            71.708
                                                             1.00 38.00
                                                                                     0
ATOM
              0
                  LYS A
                           3
                                   59.954
                                                     34.735
MOTA
          10
              CB
                  LYS A
                           3
                                   58.899
                                            70.403
                                                     37.363
                                                             1.00 39.80
                                                                                     C
MOTA
          11
              CG
                  LYS A
                           3
                                   60.157
                                            69.806
                                                     37.997
                                                             1.00 44.47
                                                                                     C
ATOM
          12
              CD
                  LYS A
                           3
                                   61.036
                                            69.120
                                                     36.954
                                                             1.00 48.61
                                                                                     C
ATOM
          13
              CE
                  LYS A
                           3
                                   61.897
                                            68.023
                                                     37.579
                                                             1.00 49.58
                                                                                     C
MOTA
          14
              N7.
                  LYS A
                           3
                                   62.832
                                            68.555
                                                     38.611
                                                             1.00 52.93
                                                                                    Ν
                                                                                    N
MOTA
          15
              Ν
                  TYR A
                           4
                                   61.206
                                            72.662
                                                     36.339
                                                             1.00 36.47
              CA
                                            72.934
                                                     35.479
                                                             1.00 36.96
                                                                                     C
MOTA
          16
                  TYR A
                           4
                                   62.351
ATOM
          17
              C
                  TYR A
                           4
                                   63.577
                                            72.172
                                                     35.977
                                                             1.00 38.55
                                                                                     C
                                                     37.096
MOTA
          18
              0
                   TYR A
                           4
                                   63.591
                                            71.670
                                                             1.00 37.91
                                                                                     0
MOTA
          19
              CB
                  TYR A
                           4
                                   62.635
                                            74.442
                                                     35.472
                                                             1.00 35.25
                                                                                     C
MOTA
          20
              CG
                  TYR A
                           4
                                   61.519
                                            75.245
                                                     34.848
                                                             1.00 34.15
                                                                                     C
              CD1 TYR A
                                                                                     C
ATOM
          21
                           4
                                   61.394
                                            75.337
                                                     33.464
                                                             1.00 32.56
                                                                                     C
MOTA
              CD2 TYR A
                                   60.554
                                            75.866
                                                     35.637
                                                             1.00 34.18
          22
                           4
                                                                                     C
ATOM
          23
              CE1 TYR A
                           4
                                   60.330
                                            76.029 32.879
                                                             1.00 33.21
                                                                                     C
MOTA
          24
              CE2 TYR A
                           4
                                   59.484
                                            76.561 35.061
                                                             1.00 33.54
MOTA
          25
              CZ
                  TYR A
                           4
                                   59.380
                                            76.637
                                                     33.684
                                                             1.00 32.10
                                                                                     C
ATOM
          26
              OH
                  TYR A
                                   58.328
                                            77.310
                                                     33.111
                                                             1.00 30.26
                                                                                     0
                           4
MOTA
          27
              N
                   TYR A
                           5
                                   64.608
                                            72.091
                                                     35.144
                                                             1.00 40.78
                                                                                     N
MOTA
          28
              CA
                  TYR A
                           5
                                   65.823
                                            71.383
                                                     35.520
                                                             1.00 42.88
                                                                                     C
ATOM
          29
              С
                   TYR A
                           5
                                   67.023
                                            72.320
                                                     35.609
                                                             1.00 44.40
                                                                                     C
MOTA
          30
              0
                   TYR A
                           5
                                   67.062
                                            73.368
                                                     34.957
                                                             1.00 44.26
                                                                                     0
MOTA
          31
              CB
                  TYR A
                           5
                                   66.104
                                            70.251
                                                     34.527
                                                             1.00 42.67
                                                                                     C
                  TYR A
ATOM
          32
              CG
                           5
                                   64.970
                                            69.255
                                                     34.423
                                                             1.00 42.51
                                                                                     C
MOTA
              CD1 TYR A
                                                                                     C
          33
                           5
                                   63.796
                                            69.579
                                                     33.745
                                                             1.00 43.00
                                                                                     C
                           5
                                   65.058
                                            67.997
                                                     35.030
                                                             1.00 43.01
MOTA
          34
              CD2 TYR A
                                                                                     C
ATOM
          35
              CE1 TYR A
                           5
                                   62.735
                                            68.682
                                                     33.670
                                                             1.00 43.13
                                                                                     С
MOTA
          36
              CE2 TYR A
                           5
                                   64.005
                                            67.090
                                                     34.963
                                                             1.00 42.79
ATOM
          37
              CZ
                  TYR A
                           5
                                   62.845
                                            67.440
                                                     34.281
                                                             1.00 43.79
                                                                                     C
                                                             1.00 42.47
ATOM
          38
              OH
                  TYR A
                           5
                                   61.794
                                            66.556
                                                     34.202
                                                                                     0
ATOM
          39
              N
                                   67:996
                                            71.934
                                                     36.429
                                                             1.00 45.72
                                                                                     N
                   ASN A
                           6
                                   69.201
                                            72.729
                                                                                     C
MOTA
          40
              CA
                  ASN A
                           6
                                                     36.636
                                                             1.00 45.99
MOTA
              С
                   ASN A
                                   70.163
                                            72.704
                                                     35.453
                                                             1.00 45.21
                                                                                     C
          41
                           6
MOTA
          42
              0
                   ASN A
                           6
                                   70.883
                                            73.673
                                                     35.218
                                                             1.00 46.34
                                                                                     0
```

ATOM	43	CB	ASN	A	6	69.926	72.243	37.893	1.00	48.66		C
ATOM	44	CG	ASN		6	69.147	72.530	39.163	1.00	51.75		С
MOTA	45		ASN		6	69.264	71.805	40.153		52.73		0
ATOM	46	ND2	ASN		6	68.356	73.601	39.147		53.06		N
MOTA	47	N	GLU		7	70.177	71.605	34.707		43.47		N
ATOM	48	CA	GLU		7	71.079	71.486	33.564	1.00	41.57		Ç
ATOM	49	С	GLU	A	7	70.346	71.136	32.284	1.00	38.29		C
ATOM	50	0	GLU	A	7	69.314	70.472	32.315	1.00	37.72		0
ATOM	51	CB	GLU	Α	7	72.127	70.393	33.817	1.00	43.70		С
ATOM	52	CG	GLU	А	7	73.090	70.645	34.973	1.00	46.76		C
ATOM	53	CD	GLU	Α	7	73.898	71.919	34.802	1.00	47.87		С
ATOM	54	OE1	GLU	A	7	74.359	72.193	33.670	1.00	49.12		0
ATOM	55	OE2	GLU	А	7	74.082	72.641	35.805	1.00	50.03		0
ATOM	56	N	PRO	A	8	70.871	71.577	31.135	1.00	35.40		N
MOTA	57	CA	PRO	Α	8	70.208	71.252	29.871	1.00	34.46		С
ATOM	58	С	PRO	Α	8	70.554	69.795	29.540	1.00	33.72		С
MOTA	59	0	PRO	Α	8	71.523	69.267	30.073	1.00	33.53		0
ATOM	6.0	CB	PRO	A	8	70.835	72.240	28.895	1.00	34.81		С
ATOM	61	CG	PRO	Α	8	72.234	72.402	29.433	1.00	33.93		C
MOTA	62	CD	PRO	Α.	8	72.018	72.481	30.923	1.00	35.69		C
ATOM	63	N	CYS	A	9	69.769	69.139	28.690	1.00	32.35		N
MOTA	64	CA	CYS	Α	9	70.080	67.760	28.330	1.00	32.79	•	C
MOTA	65	C	CYS	Α	9	71.159	67.727	27.240	1.00	30.89		С
MOTA	66	0	CYS	Α	9	71.332	68.694	26.501	1.00	30.36		0
ATOM	67	CB	CYS	A	9	68.814	67.012	27.884	1.00	35.10		С
MOTA	68	SG	CYS	A	9	67.853	67.729	26.524	1.00	42.35		S
ATOM	69	N	HIS	Α	10	71.888	66.618	27.157	1.00	30.90		N
MOTA	70	CA	HIS	Α	10	72.979	66.462	26.193	1.00	29.93		C
MOTA	71	C .	HIS	A	10	72.848	65.184	25.371	1.00	30.71		С
ATOM	72	0	HIS	Α	10	72.257	64.207	25.825	1.00	30.16		0
MOTA	73	CB	HIS	A	10	74.315	66.419	26.933	1.00	29.59		С
ATOM	74	CG	HIS	А	10	74.582	67.624	27.773	1.00	30.61		C
MOTA	75	ND1	HIS	Α	10	74.945	68.840	27.236	1.00	30.69		N
MOTA	76	CD2	HIS	Α	10	74.533	67.804	29.115	1.00	30.16		С
MOTA	77	CE1	HIS	Α	10	75.109	69.716	28.210	1.00	30.34		С
MOTA	78 -	NE2	HIS	A	10	74.864	69.112	29.359	1.00	31.65		N
ATOM	79	N	THR	Α	11	73.405	65.199	24.164	1.00	30.01		N
MOTA	80	CA	THR	Α	11	73.368	64.032	23.286	1.00	30.68		С
ATOM	81	C	THR	А	11	74.696	63.287	23.412	1.00	29.38		С
MOTA	82	0	THR	Α	11 .	75.639	63.803	24.006	1.00	29.12		0
MOTA	83	CB	THR	A	11	73.194	64.437	21.816	1.00	31.25		С
MOTA	84	OG1			11	74.303	65.251	21.419	1.00	33.58		0
MOTA	85	CG2	THR	Α	11	71.903	65.220	21.621	1.00	34.80		С
MOTA	86	N	PHE	Α	12	74.768	62.085	22.846	1.00	29.78		N
MOTA	87	CA	PHE	Α	12	75.991	61.278	22.894	1.00	31.09		С
ATOM	88	C	PHE	Α	12	77.208	61.973	22.287	1.00	31.77		С
MOTA	89	0	PHE	A	12	78.334	61.771	22.747	1.00	30.24		0
MOTA	90	CB	PHE	A	12	75.789	59.943	22.173		28.84		С
MOTA	91	ÇG	PHE	Α	12	74.853	59.003	22.877	1.00	29.84		С
MOTA	92	CD1	PHE	Α	12	74.966	58.782	24.247	1.00	28.95		C
ATOM	93	CD2	PHE	A	12	73.904	58.284	22.156	1.00	29.11		С
MOTA	94		PHE		12	74.153	57.853	24.888	1.00	30.30	•	С
ATOM	95	CE2	PHE	A	12	73.082	57.348	22.788	1.00	30.62		С
MOTA	96	CZ	PHE	A.	12	73.207	57.130	24.154	1.00	28.11		С
MOTA	97	N	ASN		13	76.984	62.770	21.243	1.00	33.09		N
MOTA	98	CA	ASN		13	78.071	63.496	20.582	1.00	33.64		С
ATOM	99	C	ASN	A	13	78.783	64.499	21.487	1.00	32.75		С

MOTA	100	0	ASN	A	13	79.884	64.944	21.168	1.00 -33.53			0
MOTA	101	CB	ASN	A	13	77.554	64.238	19.344	1.00 37.76			С
ATOM	102	CG	ASN	A	13	77.564	63.377	18.098	1.00 42.14			С
MOTA	103	OD1	ASN	A	13	78.553	62.701	17.804	1.00 46.22			0
MOTA	104	ND2	ASN	A	13	76.471	63.408	17.348	1.00 44.81			N
ATOM	105	N	GLU	A	14	78.163	64.861	22.607	1.00 31.62			N
MOTA	106	CA	GLU	A	14	78.771	65.818 .	23.531	1.00 31.09			С
MOTA	107	С	GLU	A	14	79.655	65.155	24.581	1.00 31.08			С
ATOM	108	0	GLU		14	80.097	65.801	25.527	1.00.31.33			0
MOTA	109	CB	GLU	A	14	77.684	66.629	24.232	1.00 31.42			С
ATOM	110	CG	GLU		14	76.804	67.400	23.272	1.00 32.57			С
ATOM	111	CD	GLU		14	75.692	68.138	23.971	1.00 31.00			C
MOTA	112		GLU		14	75.995	68.988	24.831	1.00 32.14			0
MOTA	113	OE2	GLU		14	74.516	67.864	23.660	1.00 32.39			0
ATOM	114	N	TYR		15	79.928	63.869	24.418	1.00 29.84			N
MOTA	115	CA	TYR		15	80.746	63.176	25.397	1.00 29.38			С
MOTA	116	С	TYR		15	81.916	62.432	24.792	1.00 29.40			C
ATOM	117	0	TYR		15	81.906	62.064	23.616	1.00 30.63			0
MOTA	118	CB	TYR		15	79.889	62.177	26.184	1.00 29.52			C
MOTA	119	CG	TYR		15		.62.805	27.147	1.00 30.93			C
ATOM	120	CD1	TYR		15	79.296	63.131	28.446	1.00 30.83			C
ATOM	121	CD2	TYR		15	77.593	63.074	26.759	1.00 30.10			G.
MOTA	122	CE1	TYR		15	78.400	63.706	29.341	1.00 32.23			C
MOTA	123	CE2	TYR		15	76.688	63.653	27.646	1.00 32.13			С
ATOM	124	CZ	TYR		15	77.099	63.967	28.934	1.00 32.37			С
MOTA	125	OH	TYR		15	76.225	64.565	29.809	1.00 35.93			0
MOTA	126-	N	LEU		16	82.929	62.216	25.620	1.00 30.01			N
MOTA	127	CA	LEU		16	84.107	61.457	25.229	1.00 30.13			С
	128	C	LEU		16	84.514	60.664	26.463	1.00 28.66			С
MOTA	129	0	LEU		16	84.207	61.048	27.592	1.00 26.73			0
MOTA	130	CB	LEU		16	85.260	62.374	24.788	1.00 31.28			С
ATOM	131	CG	LEU		16	85.169	63.110	23.440	1.00 32.96			C
MOTA	132		LEU		16	86.432	63.925	23.241	1.00 34.63			C
MOTA	133		LEU		16	85.011	62.126	22.287	1.00 33.72			С
MOTA	134	N	LEU		17	85.182	59.543	26.239	1.00 29.11			N
MOTA	135	CA	LEU		17	85.652	58.696	27.327	1.00 30.34			С
ATOM	136	С	LEU		17 .	87.129	58.990	27.618	1.00 30.21			С
ATOM	137	0	LEU		17	87.943	59.094	26.698	1.00 31.80			0
ATOM	138	CB	LEU		17	85.502	57.224	26.935	1.00 29.21			С
MOTA	139	CG	LEU		17	84.082	56.655	26.892	1.00 28.59	÷		 С
ATOM	140		LEU		17	84.051	55.435	25.990	1.00 25.58			С
ATOM	141		LEU		17	83.622	56.315	28.304	1.00 25.80			С
ATOM	142	N	ILE		18	87.466	59.144	28.892	1.00 31.07			N
ATOM	143	CA	ILE		18	88.852	59.385	29.282	1.00 30.21			C
MOTA	144	C	ΙÝΕ		18	89.418	58.024	29.677	1.00 29.84			C
MOTA	145	0	ILE		18	88.859	57.345	30.536	1.00 29.71			0
ATOM	146	CB	ILE		18	88.939	60.359	30.472	1.00 30.01		•	С
ATOM	147	CG1			18	88.464	61.748	30.035	1.00 30.69			C
ATOM	148		ILE		18	90.375	60.428	30.991	1.00 28.88			C
ATOM	149		ILE		18	88.447	62.774	31.145	1.00 31.89			С
ATOM	150	N	PRO		19	90.528	57.601	29.045	1.00 29.50			N
ATOM	151	CA	PRO		19	91.140	56.303	29.350	1.00 30.06			C
ATOM	152	C	PRO		19	91.482	56.059	30.818	1.00 29.17			C
ATOM	153	0	PRO		19	91.777	56.989	31.570	1.00 30.34			0
MOTA	154	CB	PRO		19	92.389	56.285	28.460	1.00 30.87			C
ATOM	155	CG	PRO		19	91.978	57.136	27.284	1.00 30.83			C
ATOM	156	CD	PRO	A	19	91.265	58.285	27.966	1.00 29.93			С

ATOM	157	N	GLY	Α	20	91.415	54.792	31.210	1.00 27.42		N
ATOM	158	CA	GLY	Α	20	91.745	54.398	32.566	1.00 27.95		С
MOTA	159	C	GLY	Α	20	92.936	53.469	32.445	1.00 27.30		С
ATOM	160	0	GLY	Α	20	93.543	53.402	31.386	1.00 26.88		0
ATOM	161	N	LEU		21	93.275	52.739	33.497	1.00 29.16		N
ATOM	162	CA	LEU		21	94.422	51.838	33.424	1.00 29.56		С
ATOM	163	С	LEU		21	94.130	50.584	32.611	1.00 29.75		C
ATOM	164	0	LEU		21	93.212	49.831	32.920	1.00 29.91		ō
ATOM	165	СВ	LEU		21	94.885	51.435	34.834	1.00 30.32		Č
ATOM	166	CG	LEU		21	96.026	50.403	34.888	1.00 30.63		C
ATOM	167	CD1			21	97.262	50.967	34.183	1.00 25.74	•	C
ATOM	168	CD2			21	96.342	50.047	36.348	1.00 31.08	•	C
ATOM	169	N	SER		22	94.917	50.370	31.564	1.00 31.55		N
ATOM	170	CA	SER		22	94.762	49.191	30.726	1.00 32.64		C
ATOM	171	C	SER		22	95.789	48.167	31.189	1.00 32.64		. C
ATOM		0									
	172		SER		22	96.993	48.439	31.185	1.00 32.90		0
ATOM	173	CB	SER		22	95.008	49.531	29.256	1.00 32.66		C
ATOM	174	OG	SER		22	94.090	50.505	28.793	1.00 31.63		0
ATOM	175	N	THR		23	95.305	46.998	31.600	1.00 36.61		N
ATOM	176	CA	THR		23 .	96.170	45.923	32.075	1.00 37.91		C
ATOM	177	C	THR		23	96.550	44.997	30.927	1.00 38.68		С
ATOM	178	0	THR		23	95.882	44.978	29.892	1.00 39.48		0
ATOM	179	CB	THR		23	95.478	45.107	33.174	1.00 37.72		C
MOTA	180	OG1			23	94.187	44.701	32.718	1.00 41.28		0
ATOM	181	CG2	THR		23	95.311	45.936	34.431	1.00 38.84		C
ATOM	182	N	VAL	Α	24	97.624	44.232	31.117	1.00 39.25		N
ATOM	183	CA	VAL	A	24	98.118	43.311	30.095	1.00 39.40		C
ATOM	184	C	VAL	А	24	97.105	42.274	29.611	1.00 40.18		Ç
MOTA	185	0	VAL	Α	24	97.178	41.820	28.470	1.00 39.57		0
ATOM	186	CB	VAL	Α	24	99.390	42.559	30.582	1.00 40.21		C
ATOM	187	CG1	VAL	Α	24	100.555	43.537	30.721	1.00 38.74		C
ATOM	188	CG2	VAL	А	24	99.115	41.863	31.912	1.00 40.04		C
ATOM	189	N	ASP	Α	25	96.160	41.896	30.464	1.00 41.79		N
MOTA	190	CA	ASP	A	25	95.170	40.903	30.066	1.00 45.39		С
ATOM	191	C	ASP		25	94.021	41.455	29.225	1.00 45.56		C
MOTA	192	0	ASP		25	93.233	40.684	28.681	1.00 45.92		0
ATOM	193	CB	ASP	А	25	94.592	40.185	31.294	1.00 48.41		С
ATOM	194	CG	ASP		25	93.943	41.140	32.283	1.00 51.92		С
ATOM	195		ASP		25 .	93.010	40.724	33.005	1.00 54.02		0
ATOM	196		ASP		25	94.375	42.304	32.355	1.00 53.64		0
ATOM	197	N	CYS		26	93.912	42.774	29.096	1.00 45.84		N
ATOM	198		CYS		26	92.808	43.308	28.309	1.00 45.30		C
ATOM	199	C	CYS		26	93.109	43.487	26.838	1.00 45.23		C
ATOM	200	0	CYS		26	93.730	44.463	26.426	1.00 44.99		Ö
ATOM	201	CB	CYS		26	92.301	44.641	28.867	1.00 44.12		C
ATOM	202	SG	CYS		26	90.582	45.050	28.364	1.00 43.07		s
ATOM	203	и.	ILE		27	92.663	42.521	26.049	1.00 46.24		N
ATOM	204	CA	ILE		27	92.807	42.573	24.608	1.00 47.19		C
ATOM	205	C	ILE		27	91.403	42.280	24.110	1.00 47.15		C
MOTA	206	0	ILE		27	90.651	41.553		1.00 47.43		
ATOM	207	CB	ILE		27			24.763 24.077	1.00 49.39		0 C
ATOM	207				27	93.796 93.511	41.507 40.151		1.00 49.39	•	
			ILE					24.728			C
ATOM	209		ILE		27	95.229	41.964	24.329	1.00 49.14		C
ATOM	210		ILE		27	94.444	39.039	24.270	1.00 52.58		C
ATOM	211	N	PRO		28	91.025	42.857	22.962	1.00 47.37		И
ATOM	212	CA	PRO		28	89.703	42.674	22.363	1.00 47.25		C
MOTA	213	С	PRO	A	28	89.120	41.265	22.436	1.00 47.37		С

ATOM	214	0	PRO	A	28		87.972	41.088	22.842		46.21		0
MOTA	215	CB	PRO	Α	28		89.919	43.146	20.929		48.82		C
MOTA	216	CG	PRO	Α	28		90.865	44.289	21.121		47.38		С
MOTA	217	CD	PRO	Α	28		91.866	43.722	22.111		48.12		C
MOTA	218	N	SER	Α	29		89.908	40.264	22.057		47.34		N
MOTA	219	CA	SER	A	29		89.426	38.888	22.063		46.68		C
MOTA	220	C	SER	Α	29		89.015	38.355	23.435		45.41		C
ATOM	221	0	SER		29		88.294	37.361	23.524		45.14		0
MOTA	222	CB	SER		29		90.469	37.952	21.429		48.70		C
ATOM	223	OG	SER		29		91.665	37.887	22.188		51.82		0
ATOM	224	N	ASN				89.460	38.999	24.507		43.78		N
MOTA	225	CA	ASN		30		89.079	38.528	25.832		42.85		C C
ATOM	226	С	ASN		30		87.923	39.330	26.427		40.38		0
MOTA	227	0	ASN		30		87.454	39.033	27.528		40.36		C
MOTA	228	CB	ASN		30		90.271	38.560	26.789		48.87		C
ATOM	229	CG	ASN		30		91.397	37.656	26.341		50.85		0
MOTA	230		ASN		30		91.165	36.604	25.739		50.83		N .
MOTA	231	•	ASN		30		92.629	38.052	26.644		35.43		N
ATOM	232	N	VAL		31		87.461	40.342	25.703		34.43		C
MOTA	233	CA	VAL		31		86.355	41.153 40.405	26.196 26.046		32.47		C
MOTA	234	C	VAL		31		85.030	39.858	24.990		31.37		o
ATOM '	235	O	VAL		31		.84.719 86.288	42.516			34.64		C
MOTA	236	CB	VAL		31		85.055	43.296	25.907		34.16		C
ATOM	237		VAL		31		87.554	43.325	25.763		33.50		Ċ
ATOM	238		VAL		31 32		84.262	40.376	27.125		32.26		N
MOTA	239	N	ASN		32		82.972	39.695	27.155		31.85		C
ATOM	240	CA C	ASN ASN		32	-	81.865	40.737	27.1009		31.43		C
MOTA MOTA	241 242	0	ASN		32		81.731	41.614	27.855		31.95		0
	242	CB	ASN		32		82.837	38.959	28.494		33.05		С
MOTA MOTA	243	CG	ASN		32		81.543	38.173	28.618		34.40		С
ATOM	245		ASN		32		80.616	38.330	27.826		31.77		0
ATOM	246		ASN		32		81.476	37.325	29.641		36.34		N
ATOM	247	N	LEU		33		81.070	40.638	25.944	1.00	31.73		N
ATOM	248	CA	LEU		33		79.986	41.595	25.710	1.00	31.12		С
MOTA	249	C	LEU		33		78.604	41.067	26.088	1.00	32.02		C
ATOM	250	0	LEU		33		77.582	41.607	25.661	1.00	32.34		0
ATOM	251	CB	LEU	Α	33		79.979	42.040	24.244	1.00	32.07		C
MOTA	252	CG	LEU	Α.	33		81.202	42.819	23.763	1.00	33.24		С
MOTA	253	CD1	LEU	A	33		81.030	43.165	22.300		33.95		С
MOTA	254	CD2	LEU	A	33		81.380	44.091	24.601		33.50		С
MOTA	255	· N	SER	A	34		78.574	40.003	26.878		31.24		N
MOTA	256	CA	SER	A	34		77.316	39.419	27.326		31.29		С
MOTA	257	C	SER	Α	34		76.559	40.452	28.180		30.51		С
ATOM	258	0	SER	Α	34		77.172	41.284			30.18		0
MOTA	259	CB	SER	A	34		77.613	38.154	28.136		31.20		С
MOTA	260	OG	SER	A	34		76.447	37.653	28.758		39.13		0
MOTA	261	N	THR		35		75.231	40.403	28.161		29.56		N
MOTA	262	CA	THR		35		74.445	41.364	28.923		26.77		C
MOTA	263	C	THR		35		73.013	40.869	29.167		27.05		C
MOTA	264	0	THR		35		72.435	40.168	28.336		27.90		0
MOTA	265	CB	THR		35		74.416	42.737	28.181		27.30		C
MOTA	266	OG1			35		74.121	43.788	29.110		25.66		0
ATOM	267	CG2			35		73.363	42.738	27.085		26.06		C N
MOTA	268	N	PRO		36		72.423	41.233	30.318		26.43		N C
MOTA	269	CA	PRO		36		71.058	40.815	30.653		26.22		C
MOTA	270	С	PRO	Α	36		69.955	41.534	29.866	1.00	27.39		C

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ATOM	271	0	PRO		36	70.018	42.745	29.641	1.00	26.32		0
MOTA	272	CB	PRO	Α	36	70.971	41.094	32.153	1.00	26.70		С
ATOM	273	CG	PRO	Α	36 -	71.839	42.318	32.305	1.00	25.86		С
MOTA	274	CD	PRO	Α	36	73.036	41.988	31.429	1.00	24.23		С
ATOM	275	N	LEU	Α	37	68.942	40.770	29.468	1.00	27.00		N
ATOM	276	CA	LEU		37	67.815	41.295	28.716		28.26		C
ATOM	277	C	LEU		37	66.590	41.525	29.600		29.30		C
ATOM	278	Ö	LEU		37.	65.852	42.489	29.396		29.95		
	•											0
ATOM	279	CB	LEU		37	67.444	40.334	27.580		28.03		C
MOTA	280	CG	LEU		37	66.334	40.796	26.631		27.43		C
MOTA	281		LEU		37	66.879	41.891	25.699		26.44		С
ATOM	282	CD2	LEU		37	65.821	39.615	25.813		27.22		C
ATOM	283	N	VAL	Α	38	66.375	40.650	30.583	1.00	.28.72		N
MOTA	284	CA	VAL	Α	38	65.214	40.768	31.464	1.00	27.01		C
MOTA	285	C	VAL	Α	38	65.588	40.778	32.944	1.00	28.83		C
MOTA	286	0	VAL	A·	38	66.633	40.263	33.340	1.00	30.63		0
ATOM	287	CB	VAL	A	38	64.187	39.635	31.178	1.00	28.13		C
ATOM	288	CG1	VAL		38	63.710	39.731			24,82		Ċ
MOTA	289		VAL		38	64.815	38.265	31.428		25.61		Ċ
MOTA	290	N	LYS		39	64.715	41.364	33.755		27.51		N
MOTA												
	291	CA	LYS		39	64.950	41.516	35.183		29.76		C
ATOM	292	C	LYS			.65.127	40.247	36.006		30.05		С
ATOM	293	0	LYS		39	64.584	39.196	35.684		30.31		0
MOTA	294	CB	LYS		39	63.830	42.350	35.812		29.02		Ċ
MOTA	295	CG	LYS	`A	39	62.456	41.677	35.757	1.00	29.38		C
ATOM	296	$^{\rm CD}$	LYS	Α	39	61.439	42.441	36.583	1.00	30.04		C
MOTA	297	CE	LYS	A	39	60.065	41.781	36.528	1.00	31.85		C
ATOM '	298	NZ	LYS	Α	39	59.125	42.424	37.483	1.00	31.72		N
MOTA	299	N	PHE	A	40	65.887	40.388	37.088	1.00	30.48		N
ATOM	300	CA	PHE	А	40 .	66.172	39.309	38.019		31.44		C
ATOM	301	C	PHE		40	66.417	39.922	39.392		32.56		C .
ATOM	302	0	PHE		40	66.522	41.143	39.518		33.92		0
ATOM	303	CB	PHE		40	67.411	38.516	37.575		29.74		C
ATOM	304	CG	PHE		40	68.624						
						*	39.369	37.298		28.15	•	C
ATOM	305		PHE		40	68.802	39.971	36.050		28.42		C
ATOM	306		PHE		40	69.591	39.562	38.279		27.09		C
ATOM	307		PHE		40	69.928	40.747	35.788		26.56		С
MOTA	308		PHE		40	70.723	40.336	38.031		26.08		С
MOTA	309	CZ	PHE	A	40	70.894	40.930	36.783	1.00	27.19		С
MOTA	310	N	GLN	Α	41	66.502	39.078	40.415	1.00	33.34		N
ATOM	311	CA	GLN	Α	41	66.740	39.538	41.778	1.00	35.08		C
ATOM	312	С	GLN	Α	41	68.226	39.523	42.084	1.00	32.98		C
ATOM	313	0	GLN	A	41	68.999	38.848	41.411	1.00	32.25		0
MOTA	314	CB	GLN	Α	41	66.039	38.624	42.797	1.00	38.64		С
MOTA	315	CG	GLN		41	64.528	38.606	42.729		45.39		C
ATOM	316	CD	GLN		41	63.918	39.959	43.043		48.32		Ċ
MOTA	317		GLN		41	64.168	40.538	44.105		51.57		0
MOTA	318		GLN		41	63.113	40.469	42.122		49.79		N
ATOM	319	N	LYS		42	68.605				32.94		
							40.268	43.116				N
MOTA	320	CA	LYS		42	69,985	40.341	43.580		34.24		C
ATOM	321	C	LYS		42	70.530	38.925	43.835		34.61		C
ATOM	322	0	LYS		42	69.847	38.083	44.429		32.73		0
MOTA	323	CB	LYS		42	70.031	41.148	44.874		35.33		C
MOTA	324	CG	LYS		42	71.390	41.217	45.521	1.00	39.95		C
ATOM	325	CD	LYS		42	71.305	41.933	46.855	1.00	42.65		С
MOTA	326	CE	LYS	A	42	72.661	42.007	47.524	1.00	44.06		C
MOTA	327	NZ	LYS	A	42	72.561	42.711	48.829	1.00	48.33		N

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MOTA	328	N	GLY		43	71.752	38.666	43.381	1.00				N
MOTA	329	CA	GLY	A	43	72.348	37.355	43.572	1.00				С
ATOM	330	C	GLY	Α	43	72.056	36.394	42.438	1.00	33.07			. C
MOTA	331	Q	GLY	A ·	43	72.717	35.365	42.301	1.00	32.56			0
ATOM	332	N	GLN	Α	44	71.066	36.726	41.618	1.00	33.56			N
ATOM	333	CA	GLN		44	70.695	35.883	40.484	1.00	33.80			С
ATOM	334	C	GLN		44 .	71.315	36.362	39.176	1.00			·	С
							•		1.00				0
ATOM	335	0	GLN.		44	72.039	37.353	39.140			*		
ATOM	336	CB	GLN		44	69.174	35.867	40.311		35.69			C
MOTA	337	CG	GLN	Α	44	68.406	35.347	41.507	1.00				С
MOTA	338	CD	GLN	А	44	66.898	35.438	41.324	1.00				С
MOTA	339	OE1	GLN	Α	44	66.135	34.847	42.093	1.00	39.88			0
MOTA	340	NE2	GLN	Α	44	66.461	36.186	40.310	1.00	35.88	•		N
MOTA	341	N	GLN		45	71.021	35.626	38.110	1.00	35.41			N
ATOM	342	CA	GLN		45	71.465	35.936	36.758		36.43		-	C
		C	GLN		45	70.174	36.046	35.957		34.87			C
ATOM	343							36.319		33.83			0
ATOM	344	0	GLN		45	69.170							C
MOTA	345	CB	GLN		45	72.312	34.800	36.170		40.80			
MOTA	346	CG	GLN	Α	45	73.682	34.634	36.801		46.43			C
ATOM	347	CD	GLN	A	45	74.527	35.881	36.657		50.68			C
ATOM	348	OE1	GLN	Α	45	74.757	36.360	35.543	1.00	54.30			0
ATOM	349	NE2	GLN	A	45	74.995	36.418	37.784	1.00	50.86			N
ATOM	350.	N	SER		46	70.194	36.820	34.881	1.00	32.16			N
ATOM	351	CA	SER		46	69.009	36.976	34.056	1.00	32.64			C
ATOM	352	C	SER		46	68.721	35.690	33.289		33.23			С
						69.643	35.015	32.836		32.72.			0
ATOM	353	0	SER		46					30.63			C
ATOM	354	CB	SER		46	69.204	38.120	33.059					
ATOM	355 .	OG	SER		46	68.058	38.282	32.252		30.42			0
MOTA	356	N	GLU		47	67.441	35.364	33.133		33.48			N
ATOM	357	CA	GLU	Α	47	67.047	34.167	32.399		34.97			С
ATOM	358	С	GLU	Α	47	67.453	34.269	30.936	1.00	34.59			С
ATOM	359	0	GLU	Α	47	67.588	33.261	30.251	1.00	34.40			0
ATOM	360	CB	GLU	A	47	65.536	33,963	32.492	1.00	36.97			C
ATOM	361	CG	GLU		47	65.048	33.634	33.884	1.00	40.19			С
ATOM	362	CD	GLU		47	63.541	33.663	33.982	1.00	43.59			С
ATOM	363	OE1			47	62.884	32.836	33.313		46.14			0
			GLU		47	63.010	34.519	34.726		45.57			Ō
ATOM	364						35.494	30.452		34.08			N
ATOM	365	N	ILE		48	67.633							
ATOM	366	CA	ILE		48	68.032	35.702	29.066		32.00			C
MOTA	367	C	ILE	A	48	69.188	36.698	28.991		31.52			C
MOTA	368	0	ILE	Α	48	69.075	37.847	29.418		30.71			0
MOTA	369	CB	ILE	Α	48	66.851	36.231	28.204		32.81			С
ATOM	370	CG1	ILE	Α	48	65.671,	35.254	28.264	1.00	33.69			C
MOTA	371	CG2	ILE	A	48	67.307	36.419	26.764	1.00	32.09			С
MOTA	372		ILE		48	64.439	35.718	27.503	1.00	34.71			С
ATOM	373	N	ASN		49	70.306	36.241	28.449		30.86			N
ATOM	374	CA	ASN		49	71.483	37.076	28.308		31.23			C
	375	C	ASN		49	71.892	37.131	26.851		31.45			C
ATOM													
MOTA	376	0	ASN		49 .	72.070	36.095	26.214		31.67			0
MOTA	377	CB	ASN		49	72.636	36.514	29.154		30.33			C
MOTA	378	CG	ASN		49	72.393	36.676	30.640		31.43			C
MOTA	379	OD1	ASN	Α	49	72.573	37.757	31.193	1.00	28.79			0
ATOM	380	ND2	ASN	A	49	71.958	35.602	31.292	1.00	32.52			N
MOTA	381	N	LEU		50 .	72.017	38.343	26.321	1.00	30.27			N
MOTA	382	CA	LEU		50	72.440	38.523	24.937		30.28			·C
ATOM	383	C	LEU		50	73.947	38.255	24.904		30.37			C
ATOM	384	0	LEU		50	74.624	38.437	25.916		30.24			Ō
ATON	204	•	٥٠٠٠		50	/4.024	50.457	27.710	1.00	J V . M I			~

MOTA	385	CB	LEU	A	50	72.174	39.965	24.476	1.00 28.53		С
ATOM	386	CG	LEU	Α	50	70.755	40.537	24.591	1.00 30.96		С
ATOM	387	CD1	LEU	A	50	70.767	42.022	24.227	1.00 30.43		C
MOTA	388	CD2	LEU	Α	50	69.807	39.769	23.673	1.00 30.05		С
ATOM	389	N	LYS	Α	51	74.461	37.821	23.755	1.00 30.78		N
ATOM	390	CA	LYS	Α	51	75.896	37.572	23.590	1.00 32.78	•	С
MOTA	391	C	LYS	Α	51	76.563	38.904	23.231	1.00 31.15		С
MOTA	392	0	LYS	Α	51	77.740	39.120	23.516	1.00 31.86		0
ATOM	393	CB	LYS	Α	51	76.157	36.549	22.470	1.00 33.00		C
MOTA	394	CG	LYS	Α	51	76.430	35.127	22.945	1.00 37.03		C
MOTA	395	CD	LYS	Α	51	75.265	34.540	23.694	1.00 39.28		C
MOTA	396	CE	LYS		51	75.548	33.103	24.116	1.00 42.58		С
MOTA	397	NZ	LYS		51	75.773	32.190	22.957	1.00 43.64		N
ATOM	398	N	'I L'E		52	75.802	39.777	22.571	1.00 29.58		N
MOTA	399	CA	ILE		52	76.266	41.114	22.209	1.00 28.26		C
MOTA	400	С	ILE		52	75.126	42.049	22.607	1.00 28.67		C
MOTA	401	0	ILE		52	73.954	41.700	22.476	1.00 30.64		0
MOTA	402	CB	ILE		52	76.597	41.248	20.689	1.00 29.21		C
MOTA	403	CG1	ILE		52	75.369	40.926	19.832	1.00 29.71		C
MOTA	404		ILE		52	77.768	40.317	20.326	1.00 28.36		G.
MOTA	405	CD1	ILE.		52	75.591	41.184	18.343	1.00 25.96 1.00 27.43		N
MOTA	406	N	PRO		53	75.451	43.253	23.091	1.00 27.43		C
MOTA	407	CA	PRO		53	74.436	44.217	23.521	1.00 27.31		C
MOTA	408	C	PRO		53	73.665	44.991	22.453 22.667	1.00 28.48	•	0
ATOM	409	0	PRO		53	73.321	46.152 45.140	24.431	1.00 25.91		C
ATOM	410	CB	PRO		53	75.231	45.140	23.685	1.00 27.35		C
MOTA	411	CG	PRO PRO		53	76.535 76.808	43.243	23.003	1.00 27.52		C
ATOM	412	CD			53 54	73.376	44.360	21.319	1.00 27.64		N
ATOM	413	N CA	LEU LEU		54 54	72.639	45.048	20.266	1.00 28.10		C
ATOM	414 415	CA	LEU		54 54	72.033	44.369	19.933	1.00 28.75		C
ATOM ATOM	416	0	LEU		54	71.233	43.142	19.847	1.00 29.19		0
ATOM	417	CB	LEU		54	73.486	45.135	18.989	1.00 26.86		С
ATOM	418	CG	LEU		54	74.898	45.720	19.078	1.00 27.96		С
ATOM	419	CD1			54	75.549	45.652	17.707	1.00 25.98		C
ATOM	420		LEU		54	74.857	47.159	19.584	1.00 28.24		С
ATOM	421	N	VAL		55	70.261	45.171	19.770	1.00 27.85		N
ATOM	422	CA	VAL		55	68.957	44.649	19.388	1.00 28.01		C
ATOM	423	C	VAL		55	68.426	45.554	18.276	1.00 29.53		С
ATOM	424	Ō	VAL		55	68.649	46.768	18.299	1.00 30.35		0
MOTA	425	CB	VAL		55	67.947	44.605	20.579	1.00 26.85		С
ATOM	426		VAL		55	68.531	43.797	21.725	1.00 25.48		С
MOTA	427	CG2	VAL	Α	55	67.569	45.998	21.021	1.00 26.54		С
MOTA	428	N	SER	A	56	67.765	44.961	17.284	1.00 28.53		N
MOTA	429	CA	SER	Α	56	67.224	45.735	16.174	1.00 28.75		C
ATOM	430	C	SER	Α	56	65.855	46.310	16.533	1.00 27.91		C
ATOM	431	0	SER	Α	56	65.070	45.694	17.253	1.00 29.11		0
MOTA	432	CB	SER	Α	56	67.166	44.878	14.897	1.00 28.24		С
MOTA	433	OG	SER	Α	56	66.443	43.676	15.091	1.00 30.49		0
MOTA	434	N	ALA		57	65.594	47.512	16.037	1.00 27.60		N
MOTA	435	CA	ALA		57	64.363	48.241	16.318	1.00 27.21		C
MOTA	436	С	ALA		57	63.062	47.574	15.876	1.00 29.66		C
ATOM	437	0	ALA		57	63.030	46.784	14.931	1.00 29.73		0
MOTA	438	CB	ALA		57	64.460	49.640	15.721	1.00 25.06		C
ATOM	439	N	ILE		58	61.990	47.911	16.581	1.00 28.79		N
ATOM	440	CA	ILE		58	60.660	47.379	16.302	1.00 30.03		C
ATOM	441	С	ILE	A	58	60.085	48.199	15.148	1.00 30.02		С

ATOM	442	0	ILE	A	58	59.148	48.983	15.327	1.00	30.35			0
ATOM	443	CB	ILE	A	58	59.765	47.524	17.546	1.00	28.25			С
ATOM	444	CG1	ILE		58	60.560	47.095	18.788	1.00	27.95			C
ATOM	445	CG2	ILE		58	58.508	46.677	17.390		27.16			С
ATOM	446		ILE		58	59.785	47.176	20.078	1.00				C
ATOM	447	N	MET		59	60.661	47.998	13.965	1.00				N
ATOM	448	CA	MET		59	60.275	48.743	12.772		31.82			C
		CA	MET										
ATOM	449				59	60.088	47.877	11.530		32.36			C
ATOM	450	0	MET		59	60.864	46.954	11.282		31.48			0
ATOM	451	CB	MET		59	61.341	49.799	12.479		30.41			C
ATOM	452	CG	MET		59	61.619	50.738	13.635		28.79			С
ATOM	453	SD	MET		59		51.827	13.284		31.66			S
ATOM	454	CE	MET	Α	59	62.278	52.935	12.079	1.00	26.93			C
ATOM	455	N	GLN	Α	60	59.072	48.208	10.736	1.00	34.40			И
ATOM	456	CA	GLN	Α	60	58.772	47.459	9.512	1.00	36.49			. C
ATOM	457	C	GLN	Α	60	59.974	47.433	8.582	1.00	36.55			C
ATOM	458·	0	GLN	Α	60	60.208	46.447	7.885	1.00	37.12			0
ATOM	459	CB	GLN	Α	60	57.604	48.092	8.741	1.00	36.94			С
ATOM	460	CG	GLN	Α	60	56.360	48.433	9.546	1.00	37.40			С
ATOM	461	CD	GLN		60	55.273	49.031	8.666		40.00			C
ATOM	462		GLN		60	55.562	49.808	7.753		39.70			0
ATOM	463		GLN		60	54.018	48.677	8.936		40.59		•	N
ATOM	464	N	SER		61	60.730	48.526	8.572		36.66			N
ATOM	465	CA	SER		61	61.890	48.645	7.694		36.60			C
ATOM	466	C	SER		61	63.196	48.130	8.286	-	36.12			C
ATOM	467	0	SER		61	64.274	48.388	7.738		36.48			0
ATOM	468	CB	SER		61	62.073	50.105	7.280		35.62			С
ATOM	469	OG	SER		61	62.314	50.921	8.414		41.10			0
ATOM	470	N	VAL		62	63.111	47.393	9.386		34.72			N
ATOM	471	CA	VAL	А	62	64.320	46.893	10.020	1.00	33.57			C
ATOM	472	C	VAL	А	62	64.273	45.444	10.472	1.00	33.65			C
ATOM	473	0	VAL	Α	62	65.067	44.625.	10.022	1.00	35.33			0
ATOM	474	CB	VAL	Α	62	64.692	47.757	11.253	1.00	32.43			C
ATOM	475	CG1	VAL	A	62	65.900	47.160	11.970	1.00	32.00			C
ATOM	476	CG2	VAL	А	62	64.983	49.189	10.820	1.00	32.49			С
ATOM	477	N	SER	Α	63	63.337	45.133	11.361	1.00	34.80			N
ATOM	478	CA	SER		63	63.245	43.799	11.926		34.50			С
ATOM	479	С	SER		63	62.258	42.804	11.322		35.59		7.	C
ATOM	480	0	SER		63	61.149	42.610	11.830		33.23			0
ATOM	481	CB	SER		63	62.999	43.916	13.431		33.57			C
ATOM	482	OG	SER		63	64.061	44.620	14.062	,	32.53			0
ATOM	483	N	GLY		64	62.686	42.168	10.240		36.21			N
ATOM	484	CA			64					37.02			C
			GLY			61.874	41.154	9.602					
ATOM	485	C	GLY		64	62.487	39.815	9.979		39.12	•		C
ATOM	486	0	GLY		64	63.403	39.764	10.811		36.38			0
ATOM	487	N	GLU		65	62.011	38.736	9.364		39.92			N
ATOM	488	CA	GLU		65	62.522	37.405	9.665		42.75			C
ATOM	489	С	GLU		65	64.015	37.240	9.395		42.41	•		C
ATOM	490	0	GLU		65	64.731	36.649	10.201		41.59			.0
ATOM	491	CB	GLU	A	65	61.735	36.332	8.892	1.00	46.22			C
ATOM	492	CG	GLU	A	65	61.608	36.565	7.385	1.00	51.45			C
ATOM	493	CD	GLU	A	65	60.419	37.448	7.007	1.00	55.41			C
ATOM	494	OE1	GLU	Α	65	60.438	38.668	7.305	1.00	55.84			0
ATOM	495		GLU		65	59.456	36.915	6.405		57.74		٠	0
ATOM	496	N	LYS		66	64.485	37.764	8.268		42.65			N
ATOM	497	CA	LYS		66	65.895	37.647	7.914		44.04			C
ATOM	498	C	LYS		66	66.801	38.387	8.897		41.64			C
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MOTA	499	0	LYS	Α	66	67.854	37.879	9.287	1.00	39.47		0
MOTA	500	CB	LYS	Α	66	66.132	38.169	6.494	1.00	46.38		С
MOTA	501	CG	LYS	A	66	65.289	37.488	5.415	1.00	52.36		C
MOTA	502	CD	LYS	Α	66	65.540	35.975	5.309	1.00	56.28		C
ATOM	503	CE	LYS	A	66	64.795	35.174	6.387	1.00	58.02		C
ATOM	504	NZ	LYS	А	66	64.957	33.692	6.235	1.00	57.63		N
MOTA	505	N	MET	Α	67	66.393	39.588	9.289	1.00	39.83		N
ATOM	506	CA	MET		67	67.168	40.376	10.237		37.79		C
ATOM	507	C	MET	Α	67	67.305	39.592	11.541	1.00	37.63		С
ATOM	508	Ο.	MET		67	68.409	39.413	12.061	1.00	36.92		Ο,
ATOM	509	CB	MET	A	67	66.472	41.710	10.512	1.00	37.57		C
ATOM	510	CG	MET	Α	67	67.214	42.614	11.485	1.00			С
ATOM	511	SD	MET	A	67	68.849	43.062	10.880	1.00	36.99		s
ATOM	512	CE	MET		67	68.422	44.225	9.565		34.40		С
ATOM	513	N	ALA		68	66.173	39.111	12.047		35.24		N
ATOM	514	CA	ALA		68	66.133	38.356	13.290		35.08		C
ATOM	515	C	ALA		68	67.079	37.157	13.296		35.81	•	C
ATOM	516	0	ALA		68	67.714	36.868	14.310		34.68		0
ATOM	517	CB	ALA		68	64.707	37.901	13.571		34.00		C
ATOM	518	N	ILE		69	67.169	36.460	12.167		35.92		'N.
ATOM	519	CA	ILE		69	68.043	35.298	12.063		36.63		C
ATOM	52.0	C	ILE		69	69.510	35.729	12.016		35.80		C
ATOM	521	0	ILE		69	70.344	35.204	12.754		37.14		0
ATOM	522	СВ	ILE		69	67.694	34.456	10.804	1.00	38.10		C
ATOM	523	CG1	ILE		69	66.314				39.72		
							33.814	10.982				C
ATOM	524	CG2	ILE		69	68.739	33.375	10.580		37.50		C
ATOM	525	CD1	ILE		69	65.712	33.259	9.695		40.53		C
ATOM	526	N	ALA		70	69.816	36.697	11.160		34.80		N
ATOM	527	CA	ALA		70	71.179	37.194	11.027		34.57		C
ATOM	528	C	ALA		70	71.727	37.773	12.332		34.76		C
ATOM	529	0	ALA		70	72.897	37.563	12.665		34.89		0
ATOM	530	CB	ALA		70	71.244	38.246	9.932		33.76		C
ATOM	531	N	LEU		71	70.886	38.501	13.066		34.07		N
ATOM	532	CA	LEU		71	71.315	39.113	14.318		32.78		C
ATOM	533	C	LEU		71	71.451	38.095	15.436		33.19		C
MOTA	534	0	LEU		71	72.390	38.164	16.223		32.88		0
ATOM	535	CB	LEU		71	70.348	40.223	14.737		31.82		C
MOTA	536	CG	LEU		71	70.677	41.001	16.021	1.00	31.91		C
ATOM	537	CD1	LEU		71	72.140	41.434	16.021		31.18		C
MOTA	538		LEU		71	69.758	42.226	16.127		30.99		C
MOTA	539	N	ALA		72	70.515	37.151	15.506		33.38		N
MOTA	540	CA	ALA		72	70.566	36.120	16.534		34.54		С
MOTA	541	C	ALA		72	71.820	35.272	16.354		36.16		C
ATOM	542	0	ALA		72	72.385	34.775	17.332		35.90		0
MOTA	543	CB	ALA		72	69.318	35.234	16.468		32.94		С
ATOM	544	N	ARG		73	72.242	35.103	15.102		37.20		N
ATOM	545	CA	ARG		73	73.433	34.316	14.791		40.02		С
MOTA	546	C	ARG		73	74.685	34.954	15.376		40,.27		C
ATOM	547	0	ARG		73	75.641	34.259	15.711		39.91		0
ATOM	548	CB	ARG		73	73.618	34.177	13.276		42.94		С
ATOM	549	CG	ARG		73	72.702	33.172	12.595		45.30		С
MOTA	550	CD	ARG		73	72.948	33.169	11.090		48.88		C
MOTA	551	NE	ARG		73	72.151	32.162	10.401	1.00	53.31		N
MOTA	552	CZ	ARG		73	71.960	32.126	9.084	1.00	55.75		C
MOTA	553		ARG		73	72.509	33.049	8.300	1.00	56.63		N
ATOM	554	NH2	ARG		73	71.216	31.166	8.549	1.00	56.55		N
MOTA	555	N	GLU	A	74	74.676	36.281	15.488	1.00	40.14		N

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MOTA	556	CA	GLU		74	75.819	37.003	16.025	1.00 38			С
MOTA	557	С	GLU	A	74	75.711	37.229	17.531	1.00 36	. 73		C
ATOM	558	0	GLU	A	74	76.634	37.750	18.144	1.00 37	.21		0
ATOM	559	CB	GLU	A	74	75.979	38.347	15.310	1.00 40	.15		С
ATOM	560	CG	GLU	A	74	76.113	38.239	13.796	1.00 42	.93		С
ATOM	561	CD	GLU		74	77.234	37.301	13.357	1.00 44			C
ATOM	562		GLU		74	78.397	37.518	13.762	1.00 47			0
ATOM	563	OE2			74	76.948	36.347	12.601	1.00 46			0
ATOM	564	N	GLY		75	74.586	36.851	18.127	1.00 35			N
MOTA	565	CA	GLY		75	74.436	37.026	19.562	1.00 35			C
ATOM	566	C	GLY	Α	75	73.429	38.056	20.044	1.00 35	.01		С
ATOM	567	0	GLY	A	75	73.169	38.148	21.243	1.00 34	.48		0
MOTA	568	N	GLY	Α	76	72.875	38.840	19.126	1.00 34	.39		N
ATOM	569	CA	GLY	Α.	76	71.887	39.834	19.513	1.00 33	.62		С
ATOM	570	С	GLY		76	70.483	39.299	19.281	1.00 32			C
ATOM	571	Ö	GLY		76	70.315	38.101	19.025	1.00 32			0
ATOM	572	N	ILE		77	69.475	40.165	19.374	1.00 32			N
ATOM	573	CA	ILE		77	68.096	39.735	19.151	1.00 31			C
MOTA	574	С	ILE		77	67.282	40.820	18,439	1.00 32			C
MOTA	575	0	ILE		77	67.531	42.021	18.611	1.00 31			0
ATOM	576	CB	ILE	A	77	67.400	39.369	20.484	1.00 30	.05		C
MOTA	577	CG1	ILE	Α	77	66.190	38.470	20.213	1.00 29	.38		С
ATOM.	578	CG2	ILE	Α	77	66.954	40.644	21.220	1.00 27	.82		С
MOTA	579	CD1	ILE	A	77	65.442	38.047	21.474	1.00 26	.08		C
MOTA	580	N	SER		78	66.312	40.390	17.637	1.00 32			N
ATOM	581	CA	SER		78	65.456	41.317	16.904	1.00 32			C
ATOM	582	C	SER		78	64.049	41.320	17.472	1.00 32			C
MOTA		0	SER		78							0
	583					63.592	40.322	18.016	1.00 34			
ATOM	584	CB	SER		78	65.382	40.930	15.424	1.00 30			C
ATOM	585	OG .	SER		78	66.616	41.134	14.768	1.00 30			0
MOTA	586	N	PHE		79	63.369	42.453	17.351	1.00 32			N
MOTA	587	CA	PHE	A	79	61.998	42.562	17.816	1.00 31	.78		C
MOTA	588	C	PHE	A	79	61.105	42.740	16.596	1.00 31	.81		C
ATOM	589	0	PHE	Α	79	60.896	43.854	16.130	100 33	.21		0
MOTA	590	CB	PHE	A	79	61.830	43.747	18.780	1.00 30	.40		C
MOTA	591	CG	PHE		79	62,408	43.500	20.145	1.00 29	.75	•	C
ATOM	592		PHE		79	63.754	43.732	20.401	1.00 31			C
ATOM	593		PHE		79	61.611	42.994	21.169	1.00 30			C
ATOM	594		PHE		79		43.462		1.00 30			C
			PHE			64.302		21.663				
ATOM	595				79	62.145	42.719	22.428	1.00 29			C
ATOM	596	CZ	PHE		79	63.490	42.953	22.676	1.00 30			C
ATOM	597	N	ILE		80	60.603	41.628	16.071	1.00 32			И
MOTA	598	CA	ILE	Α	80	59.726	41.651	14.902	1.00 32	.86		C
ATOM	599	C	ILE	A	80	58.677	42.748	15.075	1.00 32	.33		С
MOTA	600	0	ILE	Α	80	57.963	42.781	16.084	1.00 32	.22		0
MOTA	601	CB	ILE	A	80	59.015	40.282	14.717	1.00 32	.80		С
ATOM	602	CG1	ILE	A	80	60.056	39.175	14.529	1.00 33	.69		С
MOTA	603		ILE		80	58.082	40.329	13.508	1.00 35	.09		С
ATOM	604		ILE		80	60.974	39.387	13.347	1.00 32			C
ATOM	605	N	PHE		81	58.581	43.643	14.095	1.00 32			N
ATOM	606	CA	PHE		81	57.627	44.740	14.186	1.00 32			C
ATOM	607	C	PHE			56.188	44.274	14.368	1.00 34			C
ATOM	608	0	PHE		81	55.771	43.271	13.792	1.00 33			0
MOTA	609	CB	PHE		81	57.731	45.676	12.966	1.00 33			С
MOTA	610	CG	PHE		81	57.438	45.016	11.643	1.00 34			С
MOTA	611		PHE		81	58.376	44.191	11.033	1.00 35	.21		С
MOTA	612	CD2	PHE	Α	81	56.224	45.241	10.995	1.00 36	.11		C

MOTA	613	CE1	PHE	A	81	58.113	43.600	9.791	1.00 34.85		С
MOTA	614	CE2	PHE	Α	81	55.947	44.658	9.756	1.00 36.53		С
ATOM	615	CZ	PHE	А	81	56.895	43.836	9.153	1.00 36.94		С
ATOM	616	N	GLY	Α	82	55.441	45.014	15.184	1.00 33.59		N
ATOM	617	CA	GLY	A	82	54.055	44.675	15.439	1.00 34.64		C
ATOM	618	С	GLY		82	53.078	45.472	14.596	1.00 35.83		С
MOTA	619	0	GLY		82	51.870	45.283	14.708	1.00 36.22		0
MOTA	620	N	SER	А	83	53.594	46.363	13.753	1.00 35.37		N
ATOM	621	CA	SER		83	52.744	47.173	12.886	1.00 35.72		С
MOTA	622	С	SER		83	52.379	46.393	11.618	1.00 36.39		С
MOTA	623	0	SER		83	52.701	46.791	10.496	1.00 35.68		0
ATOM	624	CB	SER		83	53.456	48.476	12.522	1.00 34.36		С
MOTA	625	OG	SER		83	54.710	48.208	11.928	1.00 35.50		0
MOTA	626	N	GLN		84	51.714	45.264	11.826	1.00 37.28		И
ATOM	627	CA	GLN		84	51.270	44.387	10.753	1.00 38.09		C
MOTA	628	С	GLN		84	50.229	43.474	11.394	1.00 38.74		C
MOTA	629	0	GLN		84	50.021	43.542	12.604	1.00 37.63	•	0
ATOM	630	CB	GLN		84	52.445	43.569	10.214	1.00 39.17		C
MOTA	631	CG	GLN		84	53.074	42.636	11.235	1.00 40.30		С
MOTA	632	CD	GLN		84	54.255	41.877	10.668	1.00 43.44		С
MOTA	633	OE1	GLN		84	54.155	41.259	9.607	1.00 45.87		0
MOTA	634	NE2	GLN		84	55.383	41.912	11.375	1.00 43.38		N
MOTA	635	N	SER		85	49.577	42.626	10.605	1.00 39.77		N
MOTA	636	CA	SER		0.0	48.556	41.739	11.163	1.00 40.71	-	С
MOTA	637	C	SER		85	49.138	40.766	12.182	1.00 41.13		С
MOTA	638	0	SER		85	50.301	40.373	12.088	1.00 41.44		. 0
MOTA	639	CB	SER		85	47.868	40.938	10.055	1.00 40.69		C
MOTA	640	OG	SER	A	85	48.608	39.771	9.743	1.00 41.94		0
MOTA	641	N	ILE		86	48.314	40.377	13:150	1.00 41.34		N
MOTA	642	CA	ILE		86	48.721	39.437	14.187	1.00 43.32		C
MOTA	643	C	ILE		86	49.213	38.134	13.552	1.00 45.69		C
MOTA	644	0	ILE		86	50.207	37.550	13.992	1.00 45.58		0
MOTA	645	CB	ILE		86	47.540	39.117	15.132	1.00 42.04		C
MOTA	646	CG1	ILE		86	47.139	40.379	15.904	1.00 42.78	•	С
ATOM	647	CG2	ILE		86	47.913	37.986	16.075	1.00 40.93		C
MOTA	648	CD1			86	45.948	40.191	16.833	1.00 40.98		. C
MOTA	649	N	GLU		87	48.511	37.690	12.513	1.00 46.91		N
ATOM	650	CA	GLU		87	48.860	36.460	11.809	1.00 48.52		C
MOTA	.651	C	GLU		87	50.201	36.612	11.104	1.00 46.94		С
ATOM	652	0	GLU		87 `	51.025	35.700	11.098	1.00 47.16		0
ATOM	653	CB	GLU		87	47.784	36.117	10.767	1.00 50.61		C
MOTA	654	CG	GLU		87	46.364	35.944	11.318	1.00 54.49		C
MOTA	655	CD	GLU		87	45.799	37.214	11.955	1.00 57.21		С
ATOM	656		GLU		87	45.896	38.300	11.337	1.00 57.37		0
ATOM	657	OE2			87	45.241	37.121	13.074	1.00 59.49		0
MOTA	658	N	SER		88	50.408	37.778	10.508	1.00 46.26		N
ATOM	659	CA	SER		88	51.637	38.064	9.778	1.00 45.86		C
MOTA	660	C	SER		88	52.865	38.124	10.692	1.00 44.29		C
MOTA	661	0	SER		88	53.921	37.584	10.363	1.00 43.79		0
MOTA	662	CB	SER		88	51.480	39.384	9.024	1.00 46.24		C
ATOM	663	OG	SER		88	52.551	39.587	8.126	1.00 50.64		0
ATOM	664	N	GLN		89	52.725	38.781	11.838	1.00 42.05		N
MOTA	665	CA	GLN		89	53.831	38.902	12.784	1.00 41.12		C
ATOM	666	C	GLN		89	54.164	37.534	13.378	1.00 40.97		C
ATOM	667	0	GLN		89	55.331	37.147	13.464	1.00 41.60		0
ATOM	668	CB	GLN		89	53.474	39.895	13.904	1.00 37.36		C
MOTA	669	CG	GLN	А	89	54.563	40.076	14.967	1.00 34.71		С

ATOM	670	CD	GLN	A	89	54.182	41.087	16.042	1.00	32.75		С
ATOM	671	OE1	GLN	Α	89	53.004	41.260	16.354	1.00	29.71		0
MOTA	672	NE2	${\tt GLN}$	A	89	55.183	41.740	16.630	1.00	30.65		N
MOTA	673	N	ALA	Α	90	53.132	36.798	13.778	1.00	41.05		N
MOTA	674	CA	ALA	A	90	53.326	35.478	14.363	1.00	40.85		С
ATOM	675	C	ALA	Α	90	54.027	34.536	13.386	1.00	40.83		C
ATOM	676	0	ALA	A	90	54.828	33.697	13.790	1.00	42.16		0
MOTA	677	CB	ALA	A	90	51.988	34.896	14.790	1.00	40.56	•	С
MOTA	678	N	ALA	A	91	53.733	34.676	12.099	1.00	40.30		N
ATOM	679	CA	ALA	A	91	54.364	33.822	11.106	1.00	41.24		С
MOTA	680	C	ALA	A	91	55.873	34.065	11.106	1.00	41.52		C
ATOM	681	0	ALA	A	91	56.661	33.124	11.032	1.00	42.19.		0
MOTA	682	CB	ALA	A	91	53.776	34.092	9.714	1.00	38.85		С
MOTA	683	N	MET	A	92	56.278	35.327	11.192	1.00	41.97		N
MOTA	684	CA	MET	A	92	57.702	35.651	11.208	1.00	42.09		С
MOTA	685	С	MET	A	92	58.386	35.064	12.438	1.00	41.02		C
ATOM	686	0	MET	А	92	59.513	34.579	12.360	1.00	40.61		0
MOTA	687	CB	MET	Α	92	57.910	37.165	11.181	1.00	42.37		С
MOTA	688	CG	MET	A	92	57.542	37.806	9.867	1.00	41.26		С
ATOM	689	SD	MET	Α	92	57.939	39.549	9.851	1.00	41.37		S
MOTA	690	CE.	MET	Α	92	56.946	40.100	8.458	1.00	41.08		C
ATOM .	691	N	VAL	Α	93	57.702	35.116	13.574	1.00	41.53		N
ATOM	692	CA	VAL	А	93	58.256	34.578	14.808	1.00	41.04		C.
MOTA	693	C	VAL	Α	93	58.434	33.077	14.645	1.00	42.35		C
ATOM	694	0	VAL	Α	93	59.480	32.524	14.979	1.00	42.28		0
MOTA	.695	CB	VAL	Α	93	57.325	34.857	16.004	1.00	41.44		С
MOTA	696	CG1	VAL	Α	93	57.777	34.058	17.222	1.00	39.20		С
ATOM	697	CG2	VAL	Α	93	57.324	36.350	16.315	1.00	39.63		С
MOTA	698	N	HIS	A	94	57.401	32.426	14.119	1.00	43.29		N
MOTA	699	CA	HIS	Α	94	57.421	30.984	13.898	1.00	43.16		С
ATOM	700	C	HIS	Α	94	58.579	30.600	12.982	1.00	42.12		C
MOTA	701	0	HIS	Α	94	59.320	29.657	13.261	1.00	41.10		0
ATOM	702	CB	HIS	Α	94	56.100	30.538	13.263	1.00	45.51		C
ATOM	703	CG	HIS	Α	94	55.983	29.056	13.087	1.00	46.61		C
ATOM	704	ND1	HIS	Α	94	55.628	28.210	14.116	1.00	46.66		N
ATOM	705	CD2	HIS	Α	94	56.193	28.268	12.006	1.00	46.86		C
ATOM	706	CE1	HIS	Α	94	55.624	26.965	13.677	1.00	46.63		С
MOTA	707	NE2	HIS	A	94	55.964	26.972	12.400	1.00	47.89		N
ATOM	708	N	ALA	A	95	58.727	31.339	11.888	1.00	41.47		N
ATOM	709	CA	ALA	A	95	59.788	31.080	10.921	1.00	41.48		C
MOTA	710	С	ALA	Α .	95 ·	61.168	31.132	11.567	1.00	42.50		С
MOTA	711	0	ALA	Α	95	62.017	30.282	11.306	1.00	42.88		0
MOTA	712	CB	ALA	А	95	59.712	32.088	9.783	1.00	40.24		С
ATOM	713	N	VAL	Α	96	61.394	32.138	12.407	1.00	42.32		N
MOTA	714	CA	VAL	A	96	62.680	32.289	13.074	1.00	40.88		C
MOTA	715	C	VAL	А	96	62.923	31.140	14.049	1.00	41.55		C
ATOM	716	0	VAL	Α	96	64.011	30.566	14.086	1.00	41.75		0
MOTA	717	CB	VAL	Α	96	62.755	33.635	13.837	1.00	40.31		C
ATOM	718	CGl	VAL	Α	96	64.044	33.719	14.643	1.00	38.83		C
ATOM	719	CG2	VAL	А	96	62.684	34.787	12.849	1.00.	40.30		C
ATOM	720	N	LYS		97	61.897	30.802	14.823	1.00	42.33		N
MOTA	721	CA	LYS	А	97	61.989	29.735	15.810	1.00	44.12		С
MOTA	722	C	LYS	А	97	62.197	28.349	15.206	1.00	46.23		C
MOTA	723	0	LYS	А	97	62.787	27.475	15.843	1.00	46.86		0
ATOM	724	CB	LYS		97	60.730	29.718	16.686	1.00	43.33		C
MOTA	725	CG	LYS		97	60.484	31.004	17.471		42.58		C
ATOM	726	CD	LYS	Α	97	61.669	31.349	18.374	1.00	40.95		C

7 (T) (N)	707	αĐ	T 370	70	0.7	61 004	20 205	19.461	1.00 39.70	С
ATOM	727	CE	LYS		97	61.894	30.305			
MOTA	728	NZ	LYS		97	63.158	30.559	20.212	1.00 38.22	N
ATOM	729	N	ASN		98	61.713	28.143	13.985	1.00 48.10	N
ATOM	730	CA	ASN		98	61.844	26.842	13.338	1.00 51.26	C
ATOM	731	C	ASN		98	62.675	26.897	12.062	1.00 52.29	C ·
ATOM	732	0	ASN	A	98	62.383	26.192	11.096	1.00 53.51	0
MOTA	733	CB	ASN	A	98	60.456	26.274	13.023	1.00 52.57	C
ATOM	734	CG	ASN	Α	98	59.599	26.102	14.264	1.00 54.13	С
ATOM	735	OD1	ASN	Α	98	59.898	25.286	15.139	1.00 56.37	0
ATOM	736	ND2	ASN	Α	98	58.527	26.876	14.349	1.00 55.61	N
ATOM	737	N	PHE	Α	99	63.713	27.728	12.063	1.00 53.22	N
ATOM	738	CA	PHE		99	64.579	27.872	10.897	1.00 54.26	С
ATOM	739	С	PHE		99	65.526	26.686	10.731	1.00 54.80	С
ATOM	740	0	PHE		99	65.886	26.332	9.611	1.00 54.79	0
ATOM	741	СВ	PHE		99	65.398	29.160	11.005	1.00 53.75	· C
			PHE		99	66.234	29.457	9.786	1.00 54.18	C
ATOM	742	CG								c
ATOM	743		PHE		99	65.633	29.777	8.573	1.00 53.83	
ATOM	744		PHE		99	67.624	29.437	9.858	1.00 53.66	C
MOTA	745		PHE		99	66.404	30.075	7.447	1.00 53.53	C
ATOM	746	CE2	PHE		99	68.403	29.732	8.743	1.00 53.55	C
ATOM	747	CZ	PHE	A	99	67.792	30.052	7.534	1.00 53.92	C
MOTA	748	N	LYS	А	100	65.927	26.078	11.845	1.00 55.84	N
MOTA	749	CA	LYS	Α	100	66.848	24.940	11.809	1.00 57.08	С
ATOM	750	С	LYS	Α	100	66.159	23.588	11.633	1.00 58.33	C
MOTA	751	0	LYS	Α	100	66.811	22.546	11.722	1.00 58.42	Ò
ATOM	752	CB	LYS			67.691	24.893	13.086	1.00 55.72	С
MOTA	753	CG	LYS			68.611	26.083	13.298	1.00 55.04	С
ATOM	754	CD	LYS			69.353	25.929	14.616	1.00 53.54	- C
ATOM	755	CE	LYS			70.352	27.045	14.855	1.00 51.61	C
ATOM	756	NZ	LYS			71.015	26.867	16.172	1.00 50.36	N
ATOM	757	N			101	64.850	23.601	11.395	1.00 59.54	N
ATOM	758	CA	ALA			64.095	22.363	11.213	1.00 60.39	C
		C	ALA			64.471	21.672	9.904	1.00 60.69	C
MOTA	759						22.298	8.995	1.00 60.89	0
ATOM	760	0	ALA			65.016			1.00 60.64	· C
ATOM	761	CB	ALA			62.596	22.652	11.237		
ATOM	762	N	HIS			79.198	30.290	16.950	1.00 63.01	И
MOTA	763	CA	HIS			79.815	30.312	18.273	1.00 62.71	C
ATOM	764	C	HIS			79.103	31.282	19.214	1.00 60.87	C
ATOM	765	0	HIS			78.923	30.994	20.399	1.00 60.68	0
MOTA	766	CB	HIS			81.296	30.695	18.167	1.00 65.58	C
ATOM	7.67	CG	HIS	A	222	82.137	29.677		1.00 69.22	С
MOTA	768	ND1	HIS	Α	222	82.251	28.373	17.896	1.00 70.94	N
MOTA	769	CD2	HIS	А	222	82.903	29.769	16.346	1.00 70.61	C
ATOM	770	CE1	HIS	А	222	83.049	27.706	17.080	1.00 71.60	C
MOTA	771	NE2	HIS	Α	222	83.458	28,530	16.131	1.00 71.43	N
MOTA	772	N	ASN	Α	223	78.698	32.432	18.686	1.00 57.42	N
ATOM	773	CA	ASN			78.012	33.422	19.503	1.00 55.31	C
MOTA	774	С			223	76.518	33.511	19.219	1.00 52.14	C
MOTA	775	0	ASN			75.888	34.525	19.520	1.00 49.94	0
ATOM	776	CB	ASN			78.657	34.797	19.317	1.00 57.68	Ċ
ATOM	777	CG			223	79.984	34.925	20.050	1.00 60.74	C
MOTA	778		ASN			80.713	35.904	19.870	1.00 64.29	0
	779		ASN			80.713	33.942	20.890	1.00 64.29	N
ATOM										
ATOM	780	N			224	75.948	32.453	18.648	1.00 48.44	N
ATOM	781	CA			224	74.520	32.462	18.351	1.00 46.42	C
MOTA	782	C			224	73.699	32.516	19.631	1.00 43.23	. C
MOTA	783	0	GLÜ	A	224	74.041	31.889	20.631	1.00 42.87	0

ATOM	784	CB	GLU	Α	224	74.109	31.226	17.538	1.00 47.17		С
MOTA	785	CG	GLU	Ą	224	74.383	29.892	18.217	1.00 49.19		C
ATOM	786	CD	GLU	Α	224	73.622	28.735	17.581	1.00 50.18		C
ATOM	787	OE1	GLU	Α	224	73.410	28.755	16.346	1.00 51.65		,0
ATOM	788	OE2	GLU	A	224	73.246	27.799	18.318	1.00 49.83		0
ATOM	789	N	LEU	A	225	72.615	33.279	19.590	1.00 40.90		N
ATOM	790	CA	LEU	A	225	71.733	33.410	20.734	1.00 38.88		C
MOTA	791	C	LEU	Α	225	70.565	32.457	20.516	1.00 38.25		C
ATOM	792	0	LEU			69.747	32.664	19.621	1.00 36.15		0
MOTA	793	CB	LEU			71.232	34.851	20.848	1.00 37.76		C
MOTA	794	CG	LEU			70.380	35.166	22.077	1.00 37.49		C
MOTA	795	CD1	LEU			71.196	34.932	23.340	1.00 37.19		C
MOTA	796	CD2	LEU			69.898	36.602	22.007	1.00 36.97		
ATOM	797	N	VAL			70.492	31.416	21.341	1.00 38.35		N
MOTA	798	CA	VAL			69.435	30.415	21.215	1.00 39.11		C
MOTA	799	C	VAL			68.830	29.993	22.551	1.00 40.13		0
MOTA	800	0	VAL			69.337	30.345	23.617	1.00 40.81		C
MOTA	801	CB	VAL			69.969	29.133	20.533	1.00 38.58		C
MOTA	802		VAL			70.373	29.420	19.094	1.00 35.25 1.00 38.53		С
MOTA	803		VAL			71.154	28.595	21.326	1.00 40.83		N
ATOM	804	N			227	67.737	29.237	22.475	1.00 40.83		C
ATOM	805	CA			227	67.067	28.728	23.661	1.00 41.94		C
MOTA	806	C			227	67.601	27.323	23.970	1.00 43.87		0
MOTA	807	0			227	68.501	26.828	23.288			C
ATOM	808	CB			227	65.545	28.679	23.452	1.00 42.33 1.00 42.71		C
ATOM	809	CG			227	65.139	27.889	22.210		i	0
ATOM	810		ASP			65.753	26.838	21.924	1.00 43.47 1.00 40.79		0
MOTA	811				227.	64:185	28.314	21.525	1.00 46.79		N
MOTA	812	N			228	67.036	26.681	24.990	1.00 48.46		C
	813	CA			228	67.467	25.342	25.395	1.00 50.18		C
ATOM	814	C			228	67.336	24.291	24.287	1.00 50.18		0
MOTA	815	0			228	67.953	23.226	24.358 26.631	1.00 48.09		C
MOTA	816	CB			228	66.682	24.891	26.378	1.00 49.20		0
MOTA	817	OG			228	65.289	24.897 24.596	23.268	1.00 49.20		N
ATOM	818	N			229	66.537 66.331	23.685	22.148	1.00 51.37		C
ATOM	819	CA			229	67.229	24.081	20.984	1.00 50.93	•	C
MOTA	820	C			229 229	67.223	23.548	19.878	1.00 49.76		0
ATOM	821	O			229	64.865	23.723	21.699	1.00 53.18		C
ATOM	822	CB CG			229	63.873	23.725	22.784	1.00 55.38	**	C
ATOM	823				229	62.434	23.545	22.353	1.00 58.59	•	C
ATOM	824	CD			229	61.971	22.979	21.369			0
ATOM	825 826				. 229	61.716	24.413	23.087	1.00 58.58	•	N
ATOM	827	NE2			. 230	68.131	25.026	21.242	1.00 50.37		N
MOTA	828	CA			230	69.065	25.515	20.231	1.00 48.94		С
ATOM		CA			230	68.407	26.325	19.116	1.00 46.73	•	C
ATOM	829 830	0			230	68.991	26.513	18.048	1.00 47.20		0
ATOM ATOM	831	СВ			230	69.856	24.349	19.626	1.00 51.73		С
	832	CG			230	70.992	23.825	20.507	1.00 54.62		C
MOTA MOTA	833	CD			230	72.073	24.889	20.705	1.00 57.67		С
ATOM ATOM	834	CE			230	73.357	24.307	21.302	1.00 59.53		С
	835	NZ			230	73.161	23.692	22.653	1.00 59.91		N
MOTA	836	N N			231	67.195	26.811	19.362	1.00 45.43		N
ATOM		CA			231	66.494	27.621	18.368	1.00 43.78		C
ATOM	837 838	CA			231	66.851	29.087	18.595	1.00 41.98		C
ATOM		0			231	67.013	29.524	19.735	1.00 40.65		0
ATOM	839					64.979	27.445	18.495	1.00 45.11		C
ATOM	840	CB	AKG	, F	231	04.7/3	27.443	10.400	1.00 10.21		•

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MOTA	841	CG	ARG	A	231	64.494	26.006	18.362	1.00	46.09		С
MOTA	842	CD	ARG	Α	231	62.990	25.927	18.557	1.00	47.94		C
MOTA	843	NE	ARG	A	231	62.587	26.465	19.854	1.00	49.46		N
MOTA	844	CZ	ARG	A	231	61.326	26.555	20.273	1.00	52.08		С
MOTA	845		ARG			60.328	26.144	19.498	1.00	50.02		N
MOTA	846	NH2	ARG			61.063	27.058	21.476	1.00	53.40		N
MOTA	847	N	TYR			66.981	29.841	17.510	1.00	40.54		N
MOTA	848	CA	TYR			67.312	31.253	17.607		38.76		С
MOTA	849	C	TYR			66.284	32.005	18.451		38.33		С
MOTA	850	0	TYR			65.086	31.706	18.418		37.07		0
MOTA	851	CB	TYR			67.377	31.882	16.217		39.12		C
MOTA	852	CG	TYR			68.502	31.363	15.353		41.29		C
MOTA	853	CD1	TYR			69.821	31.371	15.809		41.57		C
ATOM	854	CD2	TYR			68.253	30.883	14.070		41.51		C
ATOM	855	CE1	TYR			70.867	30.915	15.002		43.44		C
ATOM	856	CE2	TYR			69.288	30.425	13.257		44.33		C
MOTA	857	CZ	TYR			70.591	30.444	13.727		44.76		C
MOTA	858	OH	TYR			71.612	30.003	12.913		47.05		0
ATOM	859	N	LEU			66.764	32.970	19.228		36.38 35.39		C N
ATOM ATOM	860 861	CA C	LEU			65.879 65.296	33.775 34.876	20.052 19.176		33.69		C
ATOM	862	0	LEU			65.937		18.230		33.90		0
ATOM	863	CB	LEU			66.650	35.338 34.390	21.226		35.98	•	C
ATOM	864	CG	LEU			66.395	33.765	22.602		39.07		c
ATOM	865		LEU			66.503	32.252	22.519		37.64	,	C
ATOM	866		LEU			67.384	34.325	23.616		38.75		C
ATOM	867	N	VAL			64.072	35.279	19.475		32.47		N
ATÓM	868	CA	VAL			63.433	36.334	18.710		31.96		C
ATOM	869	C	VAL			62.465	37.080	19.613		31.91		Ċ
ATOM	870	0	VAL			61.883	36.502	20.529		31.40		ō
ATOM	871	СВ	VAL			62.676	35.767	17.476		31.95		C
ATOM	872		VAL			61.402	35.048	17.913		29.55		C
ATOM ·	873	CG2	VAL	Α	234	62.371	36.888	16.498	1.00	29.80		С
ATOM	874	N	GLY	Α	235	62.319	38.375	19.366	1.00	32.16		N
ATOM	875	CA	GLY	Α	235	61.416	39.174	20.163	1.00	31.96	-	С
ATOM	876	C	GLY	Α	235	60.308	39.689	19.277	1.00	32.19		C
ATOM	877	0	GLY	Α	235	60.396	39.604	18.050	1.00	32.58		0
ATOM	878	N	ALA	Α	236	59.259	40.225	19.886	1.00	31.00		N
ATOM	879	CA	ALA	Α	236	58.154	40.746	19.109	1.00	31.50		C
MOTA	880	С	ALA	A	236	57.535	41.973	19.766	1.00	30.43		С
MOTA	881	0	ALA			57.275	41.981	20.965		32.80		0
ATOM	882	CB	ALA			57.095	39.653	18.911		32.43		С
ATOM	883	N			237	57.311	43.013	18.973		30.90		N
ATOM	884	CA			237	56.710	44.218	19.504		32.34		C
ATOM	885	C			237	55.206	44.067	19.618		32.69		C
ATOM	886	0			237	54.595	43.345	18.837		34.22		0
ATOM	887	N			238	54.607	44.723	20.606		32.45		N
ATOM	888	CA			238	53.161	44.668	20.774		32.44		C
MOTA	889	C			238	52.646	46.077	21.074		32.79		C
ATOM	890	0			238	53.422	46.976	21.400		32.08		0
ATOM	891	CB			238	52.739	43.709	21.927		33.39		C
MOTA	892		ILE			53.212	44.253	23.278		34.02		C
ATOM	893		ILE			53.309	42.320	21.686		32.20		C
ATOM ATOM	894 895	CD1			238 239	52.721 51.341	43.433 46.276	24.483 20.946		32.19 32.14		N
ATOM	896	N CA			239	50.768	47.579	20.946		31.92		C
ATOM	897	CA			239	49.769	47.462	22.358		33.41		C
721014	03/		MON	м	422	±2.103	11.404	44.330	1.00	JJ. 71		_

MOTA	898	0	ASN	A	239	49.391	46.357	22.759	1.00 32.91	C
ATOM	899	CB	ASN	A	239	50.111	48.161	19.958	1.00 32.71	C
MOTA	900	CG	ASN	Α	239	48.978	47.300	19.428	1.00 32.73	C
ATOM	901	OD1	ASN	Α	239	47.941	47.162	20.070	1.00 33.18	C
ATOM	902		ASN			49.175	46.717	18.249	1.00 31.34	N
ATOM	903	N			240	49.351	48.608	22.878	1.00 34.02	N.
ATOM	904	ÇA			240	48.414	48.658	23.989	1.00 35.67	C
ATOM	905	C			240	46.949				
							48.476	23.596	1.00 36.91	C
ATOM	906	0			240	46.061	48.629	24.435	1.00 35.65	C
ATOM	907	CB			240	48.555	49.995	24.739	1.00 34.88	C
ATOM	908	OG1			240	48.330	51.074	23.823	1.00 34.88	, C
ATOM	909	CG2			240	49.952	50.125	25.343	1.00 33.05	C
ATOM -	910	N			241	46.691	48.135	22.338	1.00 39.01	. V .
MOTA	911	CA	ARG	A	241	45.312	47.972	21.889	1.00 43.02	C
ATOM	912	C	ARG	Α	241	44.821	46.538	21.708	1.00 42.60	C
MOTA	913 [.]	0	ARG	А	241	43.926	46.093	22.429	1.00 41.68	C
ATOM	914	CB	ARG	A	241	45.087	48.752	20.588	1.00 46.62	C
ATOM	915	CG	ARG	A	241	43.702	48.546	19.976	1.00 52.95	C
ATOM	916	CD	ARG	Α	241	43.469	49.420	18.740	1.00 57.47	. Q
ATOM	917	NE	ARG			42.889	50.725	19.069	1.00 61.95	. 1
ATOM	918	CZ	ARG			43.504	51.681	19.763	1.00 63.53	
ATOM	919		ARG			44.738	51.496	20.218	1.00 64.10	N
ATOM	920		ARG			42.883	52.831	19.999	1.00 63.47	
ATOM	921	N	ASP				45.820			<i>V</i> .
						45.396		20.748	1.00 42.26	N.
ATOM	922	CA	ASP			44.974	44.450	20.473	1.00 43.86	C
ATOM	923	C	ASP			45.832	43.360	21.119	1.00 43.63	C
ATOM	924	0	ASP			45.930	42.258	20.585	1.00 44.69	C
ATOM	925	CB	ASP			44.930	44.214	18.957	1.00 43.42	
ATOM	926	CG	ASP			46.295	44.361	18.295	1.00 45.14	C
ATOM	927	OD1	ASP	А	242	47.320	44.022	18.931	1.00 44.30	
ATOM	928	OD2	ASP	Α	242	46.344	44.799	17.123	1.00 45.01	C
ATOM	929	N	PHE	Α	243	46.433	43.655	22.266	1.00 43.34	N
ATOM	930	CA	PHE	Α	243	47.298	42.686	22.939	1.00 43.11	C
ATOM	931	C	PHE	Α	243 '	46.612	41.409	23.434	1.00 43.36	C
ATOM	932	0	PHE	A	243	47.244	40.354	23.504	1.00 43.21	C
ATOM	933	CB	PHE	Α	243	48.043	43.368	24.097	1.00 40.53	C
ATOM	934	CG	PHE			47.147	43.890	25.179	1.00 38.93	C
ATOM	935		PHE			46.662	43.042	26.170	1.00 38.45	C
ATOM	936		PHE			46.795	45.236	25.216	1.00 38.69	C
ATOM	937		PHE				43.524	27.185		C
ATOM	938		PHE			45.974	45.731			C
ATOM	939	CZ				45.497	44.872		1.00 38.78	
ATOM	940	N	ARG				41.497		1.00 43.84	
ATOM	941	CA	ARG			44.598				N
ATOM		C					40.325	24.253	1.00 44.76	C
ATOM	942		ARG			44.549	39.225	23.197	1.00 44.01	C
	943	0	ARG		•	44.455	38.047	23.526	1.00 44.85	O
ATOM	944	CB	ARG			43.176	40.713	24.685	1.00 44.23	C
ATOM	945	CG	ARG			43.148	41.654	25.880	1.00 43.24	C
ATOM	946	CD	ARG			41.735	41.931	26.362	1.00 44.43	C
ATOM	947	NE	ARG			41.721	42.938	27.420	1.00 45.36	N
ATOM	948	CZ	ARG			41.970	44.231	27.224	1.00 46.55	C
ATOM	949		ARG			42.247	44.678	26.003	1.00 44.24	N
MOTA	950	NH2	ARG	A	244	41.953	45.077	28.248	1.00 45.03	N
ATOM	951	N	GLU	Α	245	44.614	39.610	21.929	1.00 44.30	N
ATOM	952	CA	GLU	A	245	44.599	38.634	20.849	1.00 45.31	C
ATOM	953	C	GLU	A	245	46.001	38.448	20.275	1.00 44.68	C
ATOM	954	0	GLU			46.363	37.358	19.826	1.00 44.64	0
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ATOM	955	CB	GLU	Α	245		43.640	39.071	19.733	1.00 48	3.37			С
MOTA	956	CG	GLU	Α	245		42.153	38.931	20.084	1.00 5	3.41			С
MOTA	957	CD	GLU	Α	245		41.647	39.993	21.059	1.00 5	7.52			С
ATOM	958	OE1	GLU				40.635	39.725	21.746	1.00 5	9.50			0
MOTA	959	OE2	GLU				42.239	41.099	21.132	1.00 5	9.64			0
ATOM	960	N	ARG				46.794	39.514	20.309	1.00 4	2.77			N
ATOM	961	CA	ARG				48.152	39.479	19.771	1.00 4				C
ATOM	962	C			246		49.163	38.714	20.629	1.00 3				C
ATOM	963	0	ARG				49.964	37.944	20.111	1.00 3				0
ATOM	964	CB	ARG				48.649	40.907	19.553	1.00 4				C
ATOM	965	CG	ARG					40.997	18.770	1.00 4				C
	966	CD	ARG					-	18.584	1.00 4				C
ATOM			ARG				50.355	42.442						
ATOM	967	NE					50.638	42.723	17.185	1.00 5				N
ATOM	968	CZ	ARG				49.723	43.062	16.287	1.00 4		•		C
ATOM	969		ARG				48.454	43.175	16.638	1.00 5				N
MOTA	970		ARG				50.076	43.269	15.031	1.00 5				N
MOTA	971	N	VAL				49.134	38.928	21.939	1.00 3				N
ATOM	972	CA	VAL				50.075	38.246	22.822	1.00 3				C
MOTA	973	С	VAL				49.977	36.716	22.746	1.00 3		•		С
ATOM	974	0	VAL				50.980	36.041	22.499	1.00 4				0
MOTA	975	CB	VAL	A	247		49.901	38.717	24.285	1.00 3	6.45	٠.	•	С
ATOM	976		VAL				50.735	37.867	25.217	1.00 3	5.80			С
MOTA	977	CG2	VAL	Α	247		50.315	40.184	24.402	1.00 3	6.49			С
MOTA	978	N	PRO	Α	248		48.770	36.148	22.955	1.00 3	9.79			N
ATOM	979	CA	PRO	A	248		48.615	34.688	22.895	1.00 3	8.65			С
MOTA	980	C	PRO	Α	248		49.149	34.104	21.588	1.00 3	7.90			С
MOTA	981	. 0	PRO	A	248		49.773	33.044	21.579	1.00 3	8.24			0
MOTA	982	CB	PRO	Α	248		47.107	34.498	23.050	1.00 4	0.03			C
MOTA	983	CG			248		46.727	35.633	23.951	1.00 3	9.42			С
ATOM	984	CD			248		47.499	36.790	23.340	1.00 3				C
ATOM	985	N			249		48.905	34.808	20.488	1.00 3				N
ATOM	986	CA			249		49.369	34.372	19.178	1.00 3				C
ATOM	987	C			249		50.899	34.403	19.100	1.00 4				C
MOTA	988	Ō			249		51.519	33.508	18.505	1.00 4				ō
ATOM	989	CB			249		48.77.7	35.257	18.103	1.00 3				C
MOTA	990	N			250		51.502	35.433	19.698	1.00 3				N
ATOM	991	CA			250		52.956	35.570	19.699	1.00 3				C
ATOM	992	C			250		53.585	34.501	20.587	1.00 3				C
ATOM	993	0			250			33.908	20.387	1.00 3				0
							54.600			1.00 3				C
ATOM	994	CB			250		53.357 53.642	36.974 38.057	20.176	1.00 3				C
MOTA	995	CG			250 -									
MOTA	996		LEU				53.046	37.699	17.772	1.00 3				C
ATOM	997		LEU				53.099	39.387	19.610	1.00 3				C
ATOM	998	N			251		52.974	34.256	21.740	1.00 4				N
ATOM	999	CA			251		53.469	33.243	22.665	1.00 4				C
ATOM	1000	C			251		53.413	31.878	21.985	1.00 4				C
MOTA	1001	0			251		54.406	31.153	21.942	1.00 4				0
MOTA	1002	CB			251		52.616	33.201	23.946	1.00 4				С
ATOM	1003		VAL				53.101	32.088	24.865	1.00 4	3.50			C
MOTA	1004	CG2	VAL	Α	251		52.691	34.543	24.653	1.00 4				C
ATOM	1005	N	GLU	A	252 .		52.243	31.537	21.451	1.00 4	5.33			N
MOTA	1006	CA	GLU	Α	252		52.055	30.268	20.759	1.00 .4	6.43			С
ATOM	1007	· C	GLU	A	252		53.068	30.096	19.629	1.00 4	4.48			С
ATOM	1008	0	GLU	Α	252		53.568	28.996	19.398	1.00 4	4.67			0
MOTA	1009	CB			252		50.634	30.172	20.183	1.00 4	9.48			С
MOTA	1010	CG			252		49.629	29.457	21.081	1.00 5				С
ATOM	1011	CD			252	,	49.072	30.334	22.188	1.00 5				C
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MOTA	1012	OFI	GLU	7	252	47.945	30.858	22.029	1.00 57.96		0
			GLU								
ATOM	1013					49.762	30.500	23.216	1.00 60.59		0
ATOM	1014	N	ALA			53.363	31.183	18.923	1.00 41.46		N
MOTA	1015	CA	ALA			54.315	31.135	17.820	1.00 39.92		С
MOTA	1016	С	ALA	A	253	55.748	30.896	18.306	1.00 39.79		С
MOTA	1017	0	ALA	А	253	56.638	30.587	17.509	1.00 39.66		0
MOTA	1018	CB	ALA	Α	253	54.239	32.421	17.009	1.00 38.59		C
ATOM	1019	N	GLY			55.971	31.046	19.609	1.00 38.49		N
ATOM	1020	CA	GLY			57.297	30.813	20.156	1.00 40.23		С
ATOM	1021	C			254	58.139	32.043	20.472	1.00 39.89		C
ATOM	1022	0	GLY			59.355	31.936	20.619	1.00 39.63		0
	1023	N	ALA			57.506	33.207	20.575	1.00 39.17		N
ATOM	1024	CA			255	58.232	34.432	20.888	1.00 38.09		C
MOTA	1025	C	ALA			58.933	34.287	22.238	1.00 36.72		С
ATOM	1026	0	ALA			58.324	33.872	23.223	1.00 35.94		0
MOTA	1027	CB	ALA	Α	255	57.276	35.612	20.916	1.00 37.70		C
ATOM	1028	N	ASP	Α	256	60.214	34.634	22.283	1.00 35.80		N
ATOM	1029	CA	ASP	Α	256	60.977	34.520	23.523	1.00 35.28		C
ATOM	1030	C	ASP	Α	256	60.809	35.725	24.437	1.00 33.72		С
MOTA	1031	0	ASP			60.921	35.610	25.656	1.00 32.72		0
MOTA	1032	CB	ASP			62.451	34.307	23.199	1.00 34.79		C
ATOM	1033	CG			256	62.682	33.041	22.404	1.00 37.41		C
ATOM	1034		ASP			62.584	31.948	23.003	1.00 38.37		0
MOTA	1035		ASP			62.944	33.137	21.185	1.00 34.51		0
MOTA	1036	N			257	60.538	36.881	23.845	1.00 32.63		N
MOTA	1037	CA			257	60.354	38.096	24.625	1.00 32.40		C
MOTA	1038	С	VAL	Α	257	59.502	39.085	23.845	1.00 31.76		C
MOTA	1039	0	VAL	Α	257	59.520	39.100	22.617	1.00 32.06		0
MOTA	1040	CB	VAL	Α	257	61.720	38.748	24.986	1.00 29.73		C
MOTA	1041	CG1	VAL			62.435	39.181	23.730	1.00 30.67		С
MOTA	1042		VAL			61.514	39.920	25.924	1.00 29.01		C
ATOM	1043	N			258	58.749	39.899	24.572	1.00 30.18		N
MOTA	1044	CA			258	57.886	40.894	23.957	1.00 31.57		C
ATOM	1045	C			258	58.308	42.286	24.405	1.00 31.09		C
ATOM	1046	0			258	59.036	42.441	25.384	1.00 31.25		0
MOTA	1047	CB			258	56.427	40.665	24.374	1.00 29.78		C
MOTA	1048	CG			258	55.852	39.263	24.175	1.00 31.14		C
ATOM	1049		LEU			54.440	39.223	24.729	1.00 33.95		C
MOTA	1050	CD2	LEU	Α	258	55.870	38.887	22.696	1.00 30.48		C
MOTA	1051	N	CYS	Α	259	57.849	43.298	23.680	1.00 31.62		N
MOTA	1052	CA	CYS	A	259	58.149	44.675	24.042	1.00 31.37	_	C
MOTA	1053	C	CYS	Α	259	57.070	45.613	23.521	1.00 30.31		C
MOTA	1054	0	CYS	Α	259	56.798	45.650	22.324	1.00 31.18		0
ATOM	1055	CB			259	59.503	45.114	23.485	1.00 28.99		C
ATOM	1056	SG			259	60.014	46.724	24.132	1.00 29.97		s
ATOM	1057	N			260	56.456	46.362	24.428	1.00 30.30		N
ATOM	1058	CA			260	55.431	47.317	24.042	1.00 31.13		
											C
ATOM	1059	C			260	56.147	48.408	23.248	1.00 33.06		C
MOTA	1060	0			260	57.157	48.959	23.693	1.00 32.27		0
ATOM	1061	CB			260	54.752	47.921	25.276	1.00 30.72		C
ATOM	1062		ILE			54.132	46.796	26.110	1.00 29.75		C
MOTA	1063	CG2	ILE	Α	260	53.695	48.946	24.851	1.00 27.83		C
MOTA	1064	CD1	ILE	Α	260	53.567	47.256	27.440	1.00.30.89		C
MOTA	1065	N	ASP	Α	261	55.620	48.701	22.068	1.00 33.30		N
MOTA	1066	CA	ASP	A	261	56.204	49.682	21.172	1.00 34.73		C
ATOM	1067	С			261	55.482	51.032	21.222	1.00 35.90		С
MOTA	1068	ō.			261	54.372	51.171	20.706	1.00 37.40		0
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MOTA	1069	CB	ASP	A	261	56.183	49.090	19.762	1.00		C
ATOM	1070	CG	ASP	Α	261	56.704	50.036	18.712	1.00	36.01	C
ATOM	1071	OD1	ASP	Α	261	57.519	50.924	19.041	1.00		0
MOTA	1072	OD2	ASP	Α	261	56.303	49.871	17.541	1.00		Ο.
ATOM	1073	N	SER	A	262	56.117	52.031	21.831	1.00		N
ATOM	1074	CA	SER	Α	262	55.504	53.354	21.946	1.00		С
MOTA	1075	C	SER	Α	262	56.538	54.453	22.172	1.00	35.72	С
ATOM	1076	0	SER	Α	262	57.599	54.203	22.748	1.00	35.63	0
MOTA	1077	CB	SER	Α	262	54.499	53.339	23.101	1.00	35.49	С
ATOM	1078	OG	SER	Α	262	53.993	54.629	23.377	1.00	35.23	0
ATOM	1079	N	SER	Α	263	56.240	55.671	21.722	1.00	34.24	N
ATOM	1080	CA	SER	Α	263	57.183	56.770	21.922	1.00	35.35	C
MOTA	1081	С	SER	Α	263	57.056	57.337	23.334	1.00	34.38	C
MOTA	1082	0	SER	Α	263	58.021	57.862	23.886	1.00	36.61	0
ATOM	1083	CB	SER	Α	263	56.982	57.876	20.873	1.00	35.88	С
ATOM	1084	OG	SER	Α	263	55.638	58.326	20.822	1.00	39.99	0
ATOM	1085	N	ASP	А	264	55.872	57.224	23.925	1.00	31.64	N
ATOM	1086	CA	ASP	Α	264	55.664	57.707	25.289	1.00	30.91	С
ATOM	1087	C.	ASP	A	264	55.128	56.564	26.155	1.00	30.07	С
MOTA	1088	0	ASP	Α	264	53.917	56.353	26.247	1.00	29.83	0
ATOM	1089	СВ	ASP			54.692	58.898	25.296	1.00	29.57	С
ATOM	1090	CG	ASP			54.281	59.325	26.706		29.79	С
ATOM	1091	OD1	ASP	A	264	54.945	58.947	27.696	1.00	27.03	0
MOTA	1092		ASP			53.283	60.057	26.824	1.00	29.07	0
ATOM	1093	N	GLY	Α	265	56.042	55.838	26.792	1.00	29.18	N
MOTA	1094	CA	GLY	Α	265	55.659	54.712	27.627	1.00	28.22	С
MOTA	1095	C	GLY	А	265	55.158	55.050	29.018	1.00	28.37	С
ATOM	1096	0	GLY	Α	265	54.689	54.169	29.736	1.00	28.80	0
ATOM	1097	N	PHE	A	266	55.258	56.317	29.407	1.00	27.17	N
MOTA	1098	CA	PHE	Α	266	54.798	56.752	30.721	1.00	28.12	C
MOTA	1099	С	PHE			53.275	56.847	30.584	1.00	29.95	С
ATOM	1100	0	PHE	A	266	52.699	57.932	30.598	1.00	29.08	0
ATOM	1101	СВ	PHE	A	266	55.415	58.117	31.048		27.00	C
ATOM	1102	CG	PHE	Α	266	55.483	58.432	32.522	1.00	28.08	С
MOTA	1103	CD1	PHE	Α	266	54.761	57.684	33.456	1.00	26.54	С
MOTA	1104	CD2	PHE	Α	266	56.259	59.502	32.973	1.00	25.82	C
ATOM	1105	CE1	PHE	Α	266	54.810	57.995	34.817		26.74	C
MOTA	1106	CE2	PHE	Α	266	56.317	59.827	34.328	1.00	24.90	C
MOTA	1107	CZ	PHE	Α	266	55.593	59.074	35.257		27.12	C
MOTA	1108	N	SER	Α	267	52.636	55.684	30.453		31.46	N
MOTA	1109	CA	SER	А	267	51.194	55.596	30.233		31.95	C
MOTA	1110	C	SER	Α	267	50.476	54.513	31.029		32.94	С
MOTA	1111	0	SER	Α	267	50.989	53.405	31.218		32.01	0
MOTA	1112	CB	SER	A	267	50.938	55.343	28.746		31.54	C
MOTA	1113	OG	SER	А	267	49.558	55.219	28.462		34.95	0
ATOM	1114	N	GLU	Α	268	49.266	54.833	31.466		33.57	N
ATOM	1115	CA	GLU	Α	268	48.460	53.887	32.214		35.39	С
ATOM	1116	С	GLU	Α	268	48.162	52.711	31.284		35.05	C
ATOM	1117	0	GĻU	A	268	47.945	51.589	31.736		35.30	0
MOTA	1118	CB	GLU	A	268	47.159	54.551	32.677		36.81	C
MOTA	1119	CG	GLU	A	268	46.306	53.672	33.576		41.82	C
ATOM	1120	CD	GLU	A	268	45.047		34.076		45.55	C
ATOM	1121	OE1	GLU	A	268	44.238	53.691	34.753		47.73	0
ATOM	1122	OE2	GLU	A	268	44.864		33.801		43.72	0
MOTA	1123	N			269	48.166		29.980		33.62	N
MOTA	1124	CA			269	47.907		29.002		35.48	C
MOTA	1125	C	TRP	A	269	48.958	50.813	29.063	1.00	34.72	С

MOTA	1126	0	TRP	A	269	48.632	49.637	28.873	1.00 35.26		0
ATOM	1127	CB	TRP	Α	269	47.858	52.502	27.584	1.00 36.38		С
ATOM	1128	CG	TRP	Α	269	46.659	53.368	27.322	1.00 41.33		C
ATOM	1129	CD1	TRP			46.656	54.711	27.068	1.00 40.88		C
ATOM	1130	CD2	TRP			45.289	52.948	27.272	1.00 42.34		С
ATOM	1131	NE1	TRP			45.372	55.150	26.861	1.00 42.36		N
		CE2	TRP			44.513	54.090	26.981	1.00 42.40		С
ATOM	1132						51.715	27.445	1.00 43.39	•	C
ATOM	1133	CE3	TRP			44.642			1.00 43.35		C
ATOM	1134	CZ2	TRP			43.122	54.039	26.858	1.00 44.43		C
MOTA	1135	CZ3	TRP			43.258	51.663	27.322			C
MOTA	1136	CH2	TRP			42.514	52.821	27.031	1.00 44.95		
ATOM	1137	N	GLN			50.216	51.176	29.313	1.00 32.85		N
MOTA	1138	CA	GLN			51.274	50.171	29.406	1.00 32.10		C
MOTA	1139	C	GLN	А	270	51.134	49.400	30.717	1.00 31.09		C
ATOM	1140	0	GLN	А	270	51.403	48.205	30.770	1.00 30.10		0
ATOM	1141 ~	CB	GLN	А	270	52.669	50.816	29.308	1.00 30.58		C
ATOM	1142	CG	GLN	Α	270	52.897	51.572	28.000	1.00 29.81		C
MOTA	1143	CD	GLN	Α	270	54.275	51.346	27.394	1.00 29.50		C
ATOM	1144	OE1	GLN	Ά	270	55.172	50.791	28.031	1.00 28.16		0
ATOM	1145	NE2	GLN	Α	270	54.448	51.789	26.156	1.00 26.58		N
ATOM	1146	N	LYS			50.712	50.085	31.775	1.00 32.98		N
MOTA	1147	CA	LYS			50.518	49.416	33.057	1.00 35.22		С
ATOM	1148	C	LYS			49.432	48.347	32.881	1.00 34.93		С
ATOM	1149	Ō	LYS			49.566	47.224	33.365	1.00 33.86		0
ATOM	1150	СВ			271	50.097	50.419	34.137	1.00 36.36		C
ATOM	1151	CG			271	49.780	49.767	35.481	1.00 39.94		C
					271	49.633	50.794	36.608	1.00 42.24		C
ATOM	1152	CD				49.393	50.095	37.951	1.00 45.21		C
ATOM	1153	CE			271			39.132	1.00 47.32		N
ATOM	1154	NZ			271	49.405	51.022		1.00 47.32		N
MOTA	1155	N			272	48.373	48.708	32.159			C
ATOM	1156	CA			272	47.257	47.807	31.897	1.00 35.34		C
ATOM .	1157	C			272	47.698	46.602	31.071	1.00 35.48 1.00 36.14		0
MOTA	1158	0			272	47.347	45.466	31.387			C
MOTA	1159	CB			272	46.109	48.545	31.157	1.00 35.04		C
MOTA	1160	CG1			272	45.467	49.565	32.101	1.00 35.36		
MOTA	1161	CG2			272	45.073	47.539	30.644	1.00 34.61		C
MOTA	1162	CD1				44.485	50.509	31.431	1.00 33.49		C
MOTA	1163	N			273	48.469	46.851	30.016	1.00 34.92		N
MOTA	1164	CA			273	48.951	45.777	29.156	1.00 34.08		C
MOTA	1165	C	THR	Α	273	49.844	44.791	29.918	1.00 34.99		C
MOTA	1166	0	THR	Α	273	49.675	43.578	29.803	1.00 36.08		0
ATOM	1167	CB	THR	Α	273	49.741	46.340	27.958	1.00 34.19		С
ATOM	1168	OG1	THR	A	273	48.888	47.192	27.188	1.00 35.97		0
MOTA	1169	CG2	THR	Α	273	50.248	45.216	27.069	1.00 32.81		C
ATOM	1170	N	ILE	Α	274	50.797	45.305	30.687	1.00 34.29		N
ATOM	1171	CA	ILE	Α	274	51.692	44.433	31.443	1.00 34.33		C
MOTA	1172	Ċ			274	50.900	43.660	32.493	1.00 35.70		, C
MOTA	1173	0			274	51.185	42.495	32.769	1.00 34.67		0
ATOM	1174	СВ			274	52.793	45.235	32.153	1.00 32.65		· C
ATOM	1175				274 ·	53.699	45.902	31.113	1.00 32.10		С
ATOM	1176				274	53.597	44.313	33.082	1.00 31.88		С
MOTA	1177				274	54.700	46.877	31.704	1.00 30.38		C
ATOM	1178	N			275	49.907	44.324	33.076	1.00 36.56		N
		CA			275	49.082	43.684	34.085	1.00 37.75		C
ATOM	1179					49.002	42.496	33.520	1.00 37.73		C
ATOM	1180	C			275			34.159	1.00 37.44		0
ATOM	1181	O N			275 276	48.230					N
MOTA	1182	N	TRP	A	276	47.791	42.649	32.316	1.00 36.76		14

MOTA	1183	CA	TRP	A	276	4	7.040	41.582	31.677	1.00	37.78		C
ATOM	1184	C	TRP	Α	276	4	7.952	40.391	31.416		39.15		C
ATOM	1185	0	TRP	А	276	4	7.535	39.238	31.545		38.18		0
MOTA	1186	CB	TRP	А	276	4	6.452	42.069	30.355		37.54		C
MOTA	1187	CG	TRP	Α	276	4	5.547	41.082	29.704		38.13		C
ATOM	1188	CD1	TRP	A	276		4.213	40.906	29.948		38.02		C
MOTA	1189	CD2	TRP				5.905	40.117	28.706		38.93		C
ATOM	1190	NE1	TRP				3.717	39.891	29.158		38.58		N
ATOM	1191	CE2	TRP				4.734	39.390	28.387		39.11		C
MOTA	1192	CE3	TRP				7.102	39.795	28.049		39.30		C
MOTA	1193	CZ2	TRP				4.724	38.360	27.439		39.42 40.69		C
MOTA	1194	CZ3	TRP				7.093	38.768	27.105		40.89		C
MOTA	1195	CH2	TRP				5.908	38.064	26.809 31.045		38.34		N
MOTA	1196	N			277		9.199	40.675	30.765		38.49		C
MOTA	1197	CA			277		0.164	39.621 38.850	32.033		40.03		C
ATOM	1198	C			277		0.704	37.634	31.995		39.95		0
MOTA	1199	O			277		1.444	40.197	30.113		38.18		C
MOTA	1200	CB CG1			277 277		1.112	40.752	28.725		37.35		C
MOTA	1201	CG1			277		2.520	39.121	30.016		36.41		C.
ATOM	1202 1203	CD1			277		2.274	41.440	28.036		35.39		C
ATOM ATOM	1203	N			278		0.656	39.556	33.152		41.65		N
MOTA	1205	CA			278		1.001	38.921	34.421		44.16		C
ATOM	1206	C			278		9.871	38.043	34.950	1.00	46.24		C
MOTA	1207	Ö			278		0.114	36.945	35.439		47.52		0
ATOM	1208	CB			278		1.350	39.977	35.472	1.00	42.76		С
ATOM	1209	CG			278		2.659	40.688	35.221	1.00	41.00		C
ATOM	1210	CD			278		3.853	39.767	35.416	1.00	40.34		C
ATOM	1211	NE			278		5.085	40.438	35.003	1.00	39.80		N
	. 1212	CZ			278		5.819	40.075	33.957	1.00	37.53		C
MOTA	1213				278	5	5.460	39.035	33.220	1.00	36.20		N
ATOM	1214	NH2	ARG	Α	278	5	6.895	40.777	33.628		37.01		И
MOTA	1215	N	GLU	Α	279	4	8.640	38.535	34.853	1.00	48.36		N
MOTA	1216	ÇA	GLU	A	279	4	7.471	37.794	35.320		50.94		С
MOTA	1217	C.	GLU	Α	279	4	17.248	36.513	34.512		50.49		C
MOTA	1218	0	GLU	A	279	4	16.799	35.500	35.045		50.81		0
MOTA	1219	CB	GLU	A	279	4	16.222	38.681	35.225		54.09		C
ATOM	1220	CG			279		14.889	37.951	35.431		60.56		C
MOTA	1221	CD	GLU	Α	. 279	4	14.637	37.514	36.874		64.23		C
ATOM	1222	OE1			279		13.642	36.788	37.106		65.99		0
MOTA	1223				. 279		15.419		37.777		66.30		N O
MOTA	1224	N			. 280		17.586		33.230		49.08		C
ATOM	1225	CA			280		17.399		32.323		48.34		C
MOTA	1226	С			280		18.596		32.246 32.061		47.43		0
ATOM	1227	0			280		48.423				50.57		C
ATOM	1228	CB			280		47.084				53.00		C
ATOM	1229	CG			280		46.280				55.48		C
ATOM	1230	CD			280		47.125 46.372				56.67		C
ATOM	1231	CE			280 280		45.161				57.35		N
ATOM	1232	NZ			281		49.805				45.34		N
ATOM	1233	N CA			281		51.012				41.45		C
MOTA MOTA	1234 1235	CA			281		51.012 51.987				40.66		C
ATOM	1235	0			281		53.025				40.87		0
ATOM	1237	CB			281		51.773				40.75		С
ATOM	1237	CG			281		50.998				40.09		С
ATOM	1239				281		50.798				40.34		C
ATON.	1433	UD 1						· - -					

ATOM	1240	CD2	TYR	Α	281		50.507	35.587	29.091	1.00 39.82		С
ATOM	1241	CE1	TYR	Α	281		50.139	33.099	27.928	1.00 39.98		C
ATOM	1242	CE2	TYR				49.841	35.484	27.877	1.00 40.22		С
ATOM	1243	CZ	TYR	Α	281		49.665	34.237	27.300	1.00 40.45		C
ATOM	1244	OH	TYR				49.032	34.127	26.089	1.00 43.40		0
ATOM	1245	N	GLY				51.679	35.165	34.440	1.00 39.75		N
ATOM	1246	CA	GLY				52.617	35.333	35.533	1.00 40.40		С
MOTA	1247	C	GLY				53.931	35.851	34.961	1.00 41.42	•	С
	1247	0	GLY				53.929	3.6.614	33.991	1.00 38.40		0
ATOM			ASP				55.053	35.433	35.541	1.00 43.07		N
ATOM	1249	N					56.369	35.863	35.074	1.00 45.04		С
ATOM	1250	CA	ASP					34.932	34.008	1.00 44.74		C
ATOM	1251	C	ASP				56.955	34.932	33.768	1.00 45.50		0
ATOM	1252	0	ASP				58.155		36.262	1.00 47.26		C
MOTA	1253	CB	ASP				57.333	35.961		1.00 47.20		Ċ
ATOM	1254	CG	ASP				56.936	37.049	37.253	1.00 52.49		0
ATOM	1255		ASP				56.921	38.243	36.865			0
ATOM	1256		ASP				56.639	36.713	38.424	1.00 53.68		
ATOM	1257	N	LYS				56.103	34.143	33.363	1.00 45.94		N
MOTA	1258	CA	LYS				56.542	33.197	32.334	1.00 46.43		C
MOTA	1259	С	LYS				56.751	33.889	30.988	1.00 44.34		C
MOTA	1260	0	LYS				57.530	33.432	30.152	1.00 45.10		0
MOTA	1261	CB	LYS	Α	284		55.510	32.067	32.182	1.00 50.03		C
MOTA	1262	CG	LYS	Α	284		55.898	30.981	31.181	1.00 54.57		C
ATOM	1263	CD	LYS	Α	284		54.819	29.892	31.055	1.00 57.10		С
MOTA	1264	CE	LYS	Α	284		53.656	30.317	30.157	1.00 58.56		С
ATOM	1265	NZ	LYS	Α	284		54.064	30.449	28.717	1.00 57.77		N
ATOM	1266	N	VAL	A	285		56.036	34.984	30.775	1.00 41.89		N
ATOM	1267	CA	VAL	Α	285		56.163	35.741	29.539	1.00 38.65		С
ATOM	1268	С	VAL	Α	285		56.865	37.052	29.870	1.00 37.26		C
ATOM	1269	0			285		56.445	37.785	30.768	1.00 36.50		0
ATOM	1270	-CB			285		54.784	36.024	28.918	1.00 38.41		C
ATOM	1271		VAL				54.935	36.904	27.681	1.00 36.80		С
ATOM	1272		VAL				54.113	34.710	28.552	1.00 37.51		C
ATOM	1273	N			286		57.947	37.332	29.151	1.00 35.95		N
MOTA	1274	CA			286		58.724	38.542	29.382	1.00 34.21		C
MOTA	1275	C			286		58.260	39.677	28.485	1.00 32.46		С
	1276	0			286		58.006	39.482	27.296	1.00 32.56		0
ATOM	1276	CB			286		60.215	38.262	29.151	1.00 34.13		C
MOTA		CG			286		60.755	37.082	29.955	1.00 34.78		C
MOTA	1278	CD			286		60.443	37.214	31.439	1.00 33.84		Ċ
MOTA	1279				286		61.080	36.077	32.238	1.00 33.85		C
ATOM	1280	CE				•	60.846	36.204	33.710	1.00 34.78		N
MOTA	1281	NZ			286			40.867	29.062	1.00 34.70	-	N
MOTA	1282	N			287		58.154		28.311	1.00 29.76		C
MOTA	1283	CA			287		57.702	42.028		1.00 29.76		C
MOTA	1284	C			287		58.419	43.317	28.697			0
ATOM	1285	0			287		58.390	43.744	29.856	1.00 29.71		C
MOTA	1286	СВ			287		56.160	42.221	28.472	1.00 28.44		
MOTA	1287		VAL				55.785	42.274	29.938	1.00 29.00		C
MOTA	1288		VAL				55.707	43.487	27.769	1.00 28.47		C
MOTA	1289	N			288		59.078	43.920	27.716	1.00 29.14		N
MOTA	1290	CA			288		59.766	45.177	27.941	1.00 28.04		C
MOTA	1291	C			288		58.759	46.288	27.721	1.00 28.71		C
MOTA	1292	0	GLY	A	. 288		57.760	46.089	27.023	1.00 29.59		0
MOTA	1293	N			289		59.007	47.454	28.310	1.00 28.36		N
MOTA	1294	CA	ALA	A	289		58.090	48.585	28.174	1.00 28.55		C
ATOM	1295	C	ALA	A	289		58.855	49.883	27.902	1.00 29.25		С
MOTA	1296	0	ALA	A	289		60.075	49.921	28.034	1.00 30.12		0

ATOM	1297	CB	ALA	A	289	57.242	48.720	29.444	1.00 26.88	C
MOTA	1298	N	GLY	Α	290	58.136	50.938	27.525	1.00 28.43	N
MOTA	1299	CA	GLY	Ą	290	58.779	52.209	27.232	1.00 28.28	C
MOTA	1300	C	GLY	Α	290	58.137	52.867	26.021	1.00 29.46	С
ATOM	1301	0	GLY	A	290	57.142	52.357	25.512	1.00 29.19	0
ATOM	1302	N	ASN	A	291	58.700	53.969	25.523	1.00 28.11	N
ATOM	1303	CA	ASN			59.918	54.586	26.053	1.00 27.63	C
ATOM	1304	C			291	59.689	55.673	27.101	1.00 27.03	С
ATOM	1305	0	ASN	A	291	58.656	56.336	27.113	1.00 26.50	0
ATOM	1306	СВ	ASN			60.723	55.200	24.902	1.00 24.57	C
ATOM	1307	CG			291	61.251	54.163	23.946	1.00 27.24	C
ATOM	1308		ASN			60.850	52.994	23.990	1.00 28.22	0
ATOM	1309		ASN			62.157	54.577	23.069	1.00 24.45	N
ATOM	1310	N			292	60.676	55.848	27.974	1.00 25.83	N
ATOM	1311	CA			292	60.634	56.884	28.996	1.00 26.30	C
ATOM	1312	С			292	62.000	57.576	29.002	1.00 26.52	C
ATOM	1313	0			292	62.943	57.082	28.376	1.00 27.26	0
ATOM	1314	СВ			292	60.286	56.304	30.399	1.00 26.90	C
ATOM	1315	CG1	ILE			61.132	55.066	30.705	1.00 27.05	C
ATOM	1316	CG2	ILE			58.801	55.967	30.458	1.00 26.39	C
MOTA	1317	CD1	ILE			62.564	55.368	31.104	1.00 28.87	C
MOTA	1318	N	VAL			62.115	58.707	29.695	1.00 26.68	N
ATOM	1319	CA	VAL			63.376	59.443	29.719	1.00 26.19	C
MOTA	1320	C	VAL			63.856	59.935	31.080	1.00 26.51	C
ATOM	1321	Ō	VAL			64.876	60.619	31.161	1.00 27.91	0
ATOM	1322	CB	VAL			63.323	60.668	28.776	1.00 26.56	C
ATOM	1323		VAL			63.327	60.216	27.331	1.00 24.86	C
ATOM	1324		VAL			62.079	61.493	29.068	1.00 25.40	C
ATOM	1325	N	ASP			63.127	59.618	32.143	1.00 26.19	N
ATOM	1326	CA			294	63.547	60.039	33.477	1.00 27.16	C
ATOM	1327	C	ASP			63.233	58.988	34.535	1.00 26.65	C
	1328	Ō	ASP			62.595	57.980	34.245	1.00 27.20	o
ATOM	1329	CB	ASP			62.909	61.388	33.860	1.00 26.43	C
ATOM	1330	CG	ASP			61.385	61.347	33.903	1.00 29.29	C
ATOM	1331		ASP			60.770	60.309	33.581	1.00 29.96	0
ATOM	1332		ASP			60.791	62.383	34.262	1.00 23.30	0
ATOM	1333	N			295	63.693	59.232	35.757	1.00 27.62	. N
ATOM	1334	CA	GLY			63.462	58.303	36.846	1.00 29.92	C
ATOM	1335	C	GLY			62.004	57.997	37.127	1.00 20.32	C
ATOM	1336	Ö	GLY			61.661	56.861	37.445	1.00 30.02	0
ATOM	1337	N.	GLU.	_		61.146	59.009	37.025	1.00 30.01	N
ATOM	1338	CA			296	59.713	58.831	37.265	1.00 32.13	C
ATOM	1339	C			296	59.111	57.859	36.263	1.00 31.32	C
ATOM	1340	0			296	58.331	56.989	36.631	1.00 29.01	0
MOTA	1341	СВ			296	58.977	60.169	37.157	1.00 35.45	C
ATOM	1342	CG			296	58.989	61.006	38.413	1.00 33.43	
MOTA	1343	CD			296	58.284	62.338	38.215	1.00 42.52	Ċ
ATOM	1344		GLU			57.151	62.350	37.669	1.00 50.17	0
ATOM	1345		GLU			58.865	63.375	38.609	1.00 50.17	0
ATOM	1346	N			297	59.471				
ATOM	1347	CA			297	58.961	58.024 57.146	34.994	1.00 29.22 1.00 29.30	N C
ATOM	1347	CA			297	59.453		33.954	1.00 29.30	
ATOM	1349	0	GLY				55.721	34.150		C
ATOM	1349	И				58.703	54.764	33.950	1.00 30.00	O N
ATOM	1350	CA			298 298	60.721	55.585 54.276	34.529	1.00 27.55	N C
ATOM	1351	CA			298 298	61.325 60.572	54.276	34.783	1.00 28.20 1.00 28.81	C
ATOM	1353	0	PHE			60.372	52.453	35.921 35.797	1.00 28.81	0
111011	1,,,	0	LUD	~	230	00.12/	J4.433	33.131	1.00 49.70	U

MOTA	1354	CB	PHE	Α	298	62.793	54.432	35.205	1.00 26.			С
MOTA	1355	CG	PHE	Α	298	63.403	53.164	35.747	1.00 27.			C
MOTA	1356	CD1	PHE	A	298	63.930	52.206	34.890	1.00 25.			C
MOTA	1357	CD2	PHE	A	298	63.380	52.895	37.112	1.00 28.			C
MOTA	1358	CE1	PHE	A	298	64.419	50.995	35.381	1.00 27.			C
MOTA	1359	CE2	PHE	Α	298	63.865	51.687	37.615	1.00 29.			C
ATOM	1360	CZ	PHE	A	298	64.385	50.732	36.745	1.00 26.			C
MOTA	1361	N	ARG			60.460	54.319	37.030	1.00 29.			N
MOTA	1362	CA	ARG			59.801	53.868	38.252	1.00 31.			C
MOTA	1363	C	ARG			58.372	53.388	38.000	1.00 31.		•	C
ATOM	1364	0	ARG			57.948	52.355	38.529	1.00 30.			0
ATOM	1365	CB	ARG			59.811	55.020	39.257	1.00 33.			C C
MOTA	1366	CG	ARG			58.887	54.867	40.443	1.00 39.			C
MOTA	1367	CD	ARG			59.563	54.163	41.591	1.00 43.			N
ATOM	1368	NE	ARG			60.787	54.835	42.029	1.00 46. 1.00 46.			C
ATOM	1369	CZ	ARG			61.578	54.359	42.989	1.00 46.			И
MOTA	1370	NHl	ARG			61.261	53.226	43.597	1.00 46.			N
ATOM	1371	NH2	ARG			62.691	54.996	43.329 37.192	1.00 40.			N
MOTA	1372	N	TYR			57.630	54.135 53.752	36.886	1.00 29.			C
ATOM	1373	CA	TYR			56.263 56.209	52.406	36.160	1.00 30.			C
ATOM	1374	C	TYR			55.416	51.538	36.510	1.00 29			0
MOTA	1375	O			300 300	55.584	54.813	36.025	1.00 28			C
MOTA	1376	CB CG			300	54.123	54.518	35.770	1.00 28			C
ATOM ATOM	1377 1378	CD1			300	53.152	54.795	36.737	1.00 27			С
ATOM	1379	CD2			300	53.712	53.960	34.562	1.00 27			С
ATOM	1379	CE1			300	51.799	54.526	36.497	1.00 28			С
ATOM	1381	CE2			300	52.368	53.687	34.314	1.00 29			C
ATOM	1382	CZ			300	51.419	53.974	35.284	1.00 28	.36		С
MOTA	1383	OH			300	50.098	53.722	35.019	1.00 28			0
ATOM	1384	N			301	57.047	52.230	35.145	1.00 29			N
ATOM		CA			301	57.037	50.970	34.416	1.00 29	.02		C
MOTA	1386	Ĉ			301	57.645	49.845	35.257	1.00 29	.33		C
ATOM	1387	0			301	57.286	48.685	35.098	1.00 30	.06		0
ATOM	1388	CB			301	57.768	51.119	33.079	1.00 25	.76		C
MOTA	1389	CG	LEU	Α	301	57.063	52.069	32.093	1.00 26	.66		C
MOTA	1390	CD1	LEU	Α	301	57.839	52.143	30.770		.87	•	С
MOTA	1391	CD2	LEU	Α	301	55.631	51.577	31.848	1.00 24	.96		C
MOTA	1392	N	ALA	Α	302	58.551	50.192	36.163	1.00 29			N
MOTA	1393	CA	ALA	A	302	59.165	49.184	37.019	1.00 31			C
MOTA	1394	C			302	58.093	48.588	37.946	1.00 31			C
MOTA	1395	0			302	57.913	47.371	38.003	1.00 31			0
MOTA	1396	CB			302	60.300	49.804	37.835	1.00 27			C
MOTA	1397	N			. 303	57.381	49.455	38.660	1.00 31			N
ATOM	1398	CA			. 303	56.327	49.016	39.565				C
MOTA	1399	С			. 303	55.221	48.296	38.811	1.00 32			C
MOTA	1400	0			303	54.541	47.442	39.381	1.00 33			0 C
MOTA	1401	CB			. 303	55.723	50.201	40.328	1.00 33			C
MOTA	1402	CG			303	56.701	50.831	41.301	1.00 36			0
MOTA	1403				303	57.613	50.123	41.785	1.00 37			0
MOTA	1404				303	56.546	52.033	41.601	1.00 39			И
MOTA	1405	N			304	55.034	48.649	37.540	1.00 31			C
ATOM	1406	CA			304	54.010	48.017	36.708	1.00 31 1.00 31		,	C
ATOM	1407	C			304	54.434	46.596	36.310 35.818	1.00 31		•	0
MOTA	1408	O			304	53.621	45.813 48.858	35.460	1.00 30			C
ATOM	1409	CB			304	53.741	46.272	36.505	1.00 30			N
ATOM	1410	N	لابذى	Α	305	55.711	40.212	30.303	1.00 31	د د .		14

MOTA	1411	CA	GLY	Α	305		56.179	44.929	36.195	1.00 31.25		С
ATOM	1412	C	GLY	Α	305		57.000	44.673	34.944	1.00 32.68		С
ATOM	1413	Ö	GLY				57.279	43.513	34.620	1.00 33.06		0
ATOM	1414	N	ALA				57.397	45.727	34.236	1.00 31.70		N
ATOM	1415	CA	ALA				58.192	45.560	33.018	1.00 31.42		C
			ALA				59.463	44.744	33.294	1.00 30.89		С
MOTA	1416	C						44.875	34.358	1.00 30.03		0
ATOM	1417	0	ALA				60.067					C
MOTA	1418	CB	ALA				58.564	46.934	32.450	1.00 30.33		
MOTA	1419	N	ASP				59.864	43.911	32.334	1.00 30.79		N
ATOM	1420	CA	ASP	Α	307		61.070	43.085	32.472	1.00 30.22		C
MOTA	1421	C	ASP	Α	307		62.337	43.837	32.044	1.00 29.80	•	C
ATOM	1422	0	ASP	Α	307		63.449	43.468	32.407	1.00 29.77		0
MOTA	1423	CB	ASP	Α	307		60.908	41.790	31.673	1.00 29.98		С
MOTA	1424	CG	ASP	A	307		59.931	40.835	32.328	1.00 31.85		C
ATOM	1425	OD1	ASP	A	307		60.267	40.310	33.407	1.00 30.41		0
ATOM	1426		ASP				58.826	40.626	31.783	1.00 32.28		0
ATOM	1427	N	PHE				62.153	44.876	31.242	1.00 28.99		N
ATOM	1428	CA	PHE			•	63.243	45.742	30.819	1.00 28.95		C
			PHE				62.560	47.025	30.362	1.00 29.95		 С
MOTA	1429							47.009	29.958	1.00 29.34		0
MOTA	1430	0			308		61.395			1.00 27.92		C
ATOM	1431	CB			308		64.141	45.087	29.742	1.00 27.32		C
MOTA	1432	CG			308		63.582	45.092	28.339		•	C
MOTA	1433		PHE				63.520	46.272	27.594	1.00 29.48		
MOTA	1434		PHE				63.193	43.894	27.729	1.00 29.25		C
MOTA	1435	CE1	PHE	Α	308		63.085	46.259	26.263	1.00 28.89		C
MOTA	1436	CE2	PHE	A	308		62.757	43.870	26.398	1.00 28.70		С
MOTA	1437	CZ	PHE	Α	308		62.704	45.056	25.664	1.00 29.12		C
ATOM	1438	N	ILE	Α	309		63.266	48.141	30.475	1.00 29.18		N
ATOM	1439	CA	ILE	Α	309		62.685	49.425	30.127	1.00 29.21		С
MOTA	1440	С			309		63.497	50.150	29.061	1.00 27.84		C
ATOM	1441	0			309		64.719	50.258	29.172	1.00 26.04		0
ATOM	1442	CB			309		62.539	50.284	31.422	1.00 27.91		C
MOTA	1443	CG1			309		61.524	49.602	32.353	1.00 26.47		C
	1444	CG2			309		62.123	51.703	31.082	1.00 27.10		С
ATOM					309		61.390	50.207	33.733	1.00 25.58		С
ATOM	1445						62.813	50.616	28.015	1.00 27.18		N
ATOM	1446	N			310				26.926	1.00 28.54		C
ATOM	1447	CA			310		63.480	51.322	27.149	1.00 27.05		C
ATOM	1448	C			310		63.537	52.827				Ö
MOTA	1449	. 0			310		62.550	53.460	27.529			C
MOTA	1450	CB			310		62.817	51.030		1.00 28.97		
MOTA	1451	CG			310		63.170	49.671	25.012	1.00 32.45		C
MOTA	1452	CD			310			49.652				C
MOTA	1453	CE	LYS	A	310			49.797		1.00 30.25		С
MOTA	1454	NZ	LYS	Α	310			51.156	22.318	1.00 30.02		N
MOTA	1455	N	ILE	Α	311		64.713	53.380	26.880	1.00 26.50		N
ATOM	1456	CA	ILE	Α	311		64.988	54.799	27.061	1.00 25.97		C
ATOM	1457	С	ILE	A	311		65.140	55.546	25.744	1.00 26.10		С
MOTA	1458	0			311		65.875	55.115	24.854	1.00 24.93		0
ATOM	1459	СВ			311		66.297	54.995	27.851	1.00 24.14		C
MOTA	1460				311		66.229			1.00 23.37		С
MOTA	1461				311		66.541	56.493	28.113	1.00 21.90		С
					311		67.585	53.999		1.00 22.04		С
MOTA	1462						64.440	56.668	25.619	1.00 27.44		N
MOTA	1463	N			312			57.453		1.00 27.41		C
ATOM	1464	CA			312		64.587			1.00 23.07		C
MOTA	1465	C			312		63.364					0
ATOM	1466	0			312		62.499					
MOTA	1467	N	ILE	A	313		63.316	59.342	23.671	1.00 34.02		N

ATOM	1468	CA	ILE	Α	313	62.242	60.063	23.005	1.00	35.18	С
MOTA	1469	С	ILE	А	313	62.860	61.264	22.294	1.00	36.95	С
MOTA	1470	0	ILE	Α	313	63.446	62.143	22.937	1.00	33.67	0
ATOM	1471	CB	ILE	Α	313	61.184	60.588	23.991	1.00	35.37	C
MOTA	1472	CG1	ILE	Α	313	60.488	59.419	24.697	1.00	37.50	С
MOTA	1473	CG2	ILE			60.161	61.420	23.236	1.00	36.43	С
MOTA	1474				313	59.485	59.848	25.762		34.44	С
ATOM	1475	N	GLY			62.744	61.280	20.968		39.08	N
ATOM	1476	CA	GLY			63.269	62.384	20.180		42.63	C
ATOM	1477	C	GLY			64.709	62.259	19.711		45.06	C
ATOM	1478	0			314	65.204	63.127			46.48	0
								18.984			
ATOM	1479	N			315	65.383	61.186	20.111		45.85	N
MOTA	1480	CA	GLY			66.767	60.997	19.716		47.36	C
ATOM	1481	C	GLY			66.970	60.175	18.456		48.37	С
ATOM	1482	0			315	68.067	60.169	17.901		48.87	. 0
MOTA	1483	N			316	65.929	59.482	18.002	1.00	49.42	N
MOTA	1484	CA			316	66.042	58.666	16.802	1.00	50.45	C
ATOM	1485	C	GLY	Α	316	66.512	59.444	15.581	1.00	52.07	C
MOTA	1486	0	GLY	Α	316	66.307	60.655	15.492		51.74	0
MOTA	1487	N	SER	Α	317	67.137	58.748	14.634	1.00	53.21	· N
ATOM	1488	CA	SER	Α	317	67.640	59.384	13.417	1.00	55.05	C
MOTA	1489	C	SER	A	317	66.513	59.886	12.519	1.00	56.78	С
MOTA	1490	0			317	66.689	60.855	11.782		57.20	0
MOTA	1491	СВ			317	68.529	58.413	12.629	1.00	53.62	C
ATOM	1492	OG			317	67.769	57.378	12.034		52.76	Ö
ATOM	1493	N·			318	65.360	59.226	12.575		59.64	N
ATOM	1494	CA			318	64.210	59.634	11.770		63.21	C
ATOM	1495	C	•		318	63.236	60.457	12.599		65.18	C
ATOM	1496	0			318	62.033	60.454	12.337		66.41	0
ATOM	1497	CB			318	63.425	58.425	11.193		62.53	C
ATOM	1498		ILE			62.907	57.531	12.325		61.87	C
ATOM	1499		ILE			64.292	57.668	10.216		63.60	C
ATOM	1500	CD1	ILE			63.986	56.875	13.169		63.20	С
HETATM		N			319	63.755	61.160	13.601		67.42	N
HETATM		CA			319	62.906	61.974	14.457		69.97	С
HETATM		CB			319	62.908	61.424	15.883		69.24	C
HETATM	1504	SG			319	61.855	62.386	17.013	1.00	71.47	S
HETATM	1505	C			319	63.286	63.449	14.489		71.57	С
HETATM	1506	0	CSO	A	319	64.383	63.812	14.916	1.00	71.62	0
HETATM	1507	OD	CSO	А	319	60.102	62.492	16.543	1.00	68.93	0
ATOM	1508	N	ILE	Α	320	62.363	64.292	14.035	1.00	73.78	N
ATOM	1509	CA	ILE	Α	320	62.568	65.736	14.026	1.00	75.95	C
-ATOM	1510	С	ILE	A	320	61.613	66.330	15.064	1.00	77.00	С
MOTA	1511	0	ILE	Α	320	60.712	67.099	14.730	1.00	77.56	0
MOTA	1512	CB			320	62.250	66.346	12.636		76.42	·C
MOTA	1513		ILE			62.907	65.512	11.529		76.94	C
ATOM	1514		ILE			62.740	67.793	12.577		76.02	c
ATOM	1515		ILE			64.419	65.396	11.639		77.38	Ċ
ATOM	1516	N			321	61.821	65.948	16.322		78.28	N
ATOM	1517	CA			321	61.000	66.397	17.448		79.55	C
ATOM	1518	C			321	60.432	67.809	17.303		79.96	C
ATOM	1519	0			321	59.222	68.014	17.421		79.36	0
ATOM	1520	CB			321	61.798	66.340	18.767		79.97	C
ATOM	1521		THR			62.325	65.020	18.951		80.89	0
ATOM	1522		THR			60.902	66.688	19.942		79.20	С
ATOM	1523	N			322	61.312	68.776	17.057		80.56	N
MOTA	1524	CA	ARG	A	322	60.911	70.173	16.903	1.00	81.44	C.

ATOM	1525	С	ARG	Α	322	60.282	70.402	15.533	1.00	80.96	C
MOTA	1526	0	ARG	Α	322	60.658	71.317	14.796	1.00	81.59	0
ATOM	1527	CB	ARG	Α	322	62.128	71.076	17.090	1.00	82.63	C
ATOM	1528	CG	ARG	Α	322	62.904	70.739	18.345	1.00	84.75	C
MOTA	1529	CD	ARG	Α	322	64.194	71.520	18.459	1.00	85.81	C
MOTA	1530	NE	ARG			65.052	70.945	19.491	1.00		N
ATOM	1531	CZ			322 .	66.238	71.432	19.834	1.00		C
ATOM	1532		ARG			66.711	72.512	19.226	1.00		N
							70.831	20.775	1.00		N
ATOM	1533		ARG			66.955					
ATOM	1534	N			323	59.318	69.549	15.211	1.00		N
ATOM	1535	CA			323	58.595	69.596	13.949	1.00		C
MOTA	1536	C			323	57.395	68.679	14.153	1.00		C
MOTA	1537	0			323	56.482	68.618	13.328	1.00		0
MOTA	1538	CB			323	59.485	69.078	12.818	1.00		С
MOTA	1539	CG	GLU	А	323′	58.886	69.206	11.429	1.00	82.04	. С
MOTA	1540	CD	GLU	A	323	59.856	68.784	10.341	1.00	83.25	C
ATOM	1541	OE1	GLU	Α	323	60.262	67.601	10.328	1.00	84.45	0
MOTA	1542	OE2	GLU	Α	323	60.216	69.638	9.501	1.00	83.53	0
ATOM	1543	N	GLN	Α	324	57.419	67.969	15.278	1.00	73.73	N
ATOM	1544	CA			324	56.358	67.047	15.656	1.00	70.84	С
ATOM	1545	C			324	55.584	67.624	16.841	1.00		С
ATOM	1546	0			324	54.752	68.516	16.665	1.00		0
ATOM	1547	CB			324	56.951	65.684	16.028	1.00		c
ATOM	1548	CG			324	57.667	64.984	14.883	1.00		c
		CD					64.622	13.740	1.00		C
ATOM	1549				324	56.732					0
ATOM	1550		GLN			56.070	65.485	13.162	1.00		
ATOM	1551	NE2			324	56.678	63.338	13.407	1.00		N
MOTA	1552	N			325	55.865	67.129	18.045	1.00		N
MOTA	1553	CA			325	55.169	67.608	19.237	1.00		C
MOTA	1554	C			325	56.069	68.271	20.273	1.00		С
MOTA	1555	0	LYS	A	325	55.592	68.754	21.301	1.00		0
MOTA	1556	CB	LYS	Α	325	54.387	66.466	19.894	1.00	58.47	C
MOTA	1557	CG	LYS	Α	325	53.233	65.959	19.042	1.00	57.42	C
MOTA	1558	CD	LYS	A	325	52.221	65.177	19.862	1.00	57.29	С
MOTA	1559	CE	LYS	Α	325	52.836	63.949	20.508	1.00	55.50	C
MOTA	1560	NZ	LYS	Α	325	51.779	63.110	21.124	1.00	55.85	N
MOTA	1561	N	GLY	Α	326	57.369	68.292	20.005	1.00	49.91	N
MOTA	1562	CA	GLY	Α	326	58.288	68.924	20.929	1.00	46.08	C
ATOM	1563	С			326	58.462	68.239	22.271	1.00	44.72	C
ATOM	1564	0			326	58.571	68.909	23.300	1.00		0
ATOM	1565	N			327		66.908	22.269	1.00		. N
ATOM	1566	CA			327	58.676	66.151		1.00		C
ATOM	1567	C			327	59.998	65.398	23.351	1.00		C
MOTA	1568				327	60.387	65.011	22.248		39.17	o
		O			327				1.00		C
ATOM	1569	CB				57.526	65.136	23.764	1.00		C
ATOM	1570				327	57.530	64.026	22.713			
ATOM	1571				327	56.179	65.859	23.752	1.00		C
ATOM	1572				327	56.507	62.920	22.986	1.00		C
ATOM	1573	N			328	60.706	65.206	24.455	1.00		N
MOTA	1574	CA			328	61.963	64.490	24.362	1.00		C
MOTA	1575	C			328	63.040	64.952	25.321	1.00		C
MOTA	1576	0	GLY	A	328	62.810	65.790	26.201		33.46	0
ATOM	1577	N			329	64.233	64.399	25.132		35.76	N
MOTA	1578	CA	ARG	Α	329	65.361	64.723	25.981		34.21	C
ATOM	1579	C	ARG	Α	329	66.625	64.178	25.333	1.00	32.60	C
ATOM	1580	0	ARG	Α	329	66.592	63.117	24.719	1.00	33.20	0
ATOM	1581	CB			329	65.152	64.070	27.353	1.00	34.78	C

	1500	00	NDC	70	220	66.083	64.550	28.441	1 00	32.95		C
MOTA	1582		ARG .							32.61		Ċ
MOTA	1583		ARG			65.843	63.788	29.726				N
MOTA	1584	NE	ARG			66.249	64.578	30.881		32.32		
ATOM	1585	CZ	ARG	Α	329	66.174	64.166	32.142		33.26		C
MOTA	1586	NH1	ARG	Α	329	65.708	62.956	32.431	1.00	31.12		Ŋ
MOTA	1587	NH2	ARG	Α	329	66.561	64.975	33.118	1.00	34.83		N
ATOM	1588	N	GLY			67.733	64.908	25.452	1.00	32.13		N
	1589	CA	GLY			68.978	64.419	24.893		29.42		C
MOTA						69.146	62.988	25.382		27.97	•	. C
MOTA	1590	С	GLY							26.61		Ö
MOTA	1591	0	GLY			68.986	62.718	26.569				N
MOTA	1592	N	GLN			69.455	62.076	24.469		28.50		
MOTA	1593	CA	GLN	Α	331	69.611	60.667	24.801		28.43		C
MOTA	1594	C	GLN	Α	331	70.586	60.394	25.947	1.00	28.88		C
MOTA	1595	0	GLN	Α	331	70.294	59.570	26.819	1.00	29.14		0
ATOM	1596	CB	GLN			70.049	59.876	23.561	1.00	28.74		C
ATOM	1597	CG	GLN			69.975	58.362	23.734	1.00	30.37		C
	1598	CD	GLN			68.540	57.846	23.795	1.00	34.54		С
ATOM						68.288	56.727	24.250		34.07		0
MOTA	1599		GLN				58.655	23.324		32.56		N
MOTA	1600		GLN			67.596				26.91		N
MOTA	1601	N	ALA			71.733	61.073	25.951				
MOTA	1602	CA ·	ALA			72.732	60.857			27.04		 C
MOTA	1603	С	ALA	A	332	72.165	61.146	28.389		26.51		C
MOTA	1604	0	ALA	Α	332	72.235	60.304	29.289		24.75		0
MOTA	1605	CB	ALA	Α	332	73.981	61.725	26.743	1.00	26.35		C
ATOM	1606	N	THR			71.602	62.337	28.555	1.00	25.80		N
ATOM	1607	CA	THR			71.021	62.735	29.828	1.00	26.22		C
		C	THR			69.921	61.763	30.251		26.29		С
MOTA	1608						61.427	31.430		24.39		Ō
MOTA	1609	0	THR			69.798		•		27.31		C
MOTA	1610	CB	THR			70.421	64.145	29.740				0
MOTA	1611	OG1	THR			71.440	65.071	29.336		28.44		
MOTA	1612	CG2	THR	A	333	69.863	64.566	31.094		27.55		,C
ATOM	1613	N	ALA	Α	334	69.128	61.321	29.276		25.58		N
MOTA	1614	CA	ALA	Α	334	68.040	60.384	29.520	1.00	25.32		C
ATOM	1615	C	ALA	A	334	68.570	59.079	30.125	1.00	24.79		C
MOTA	1616	0	ALA	Α	334	68.064	58.603	31.146	1.00	24.60		0
ATOM	1617	СВ	ALA			67.303	60.094	28.210	1.00	24.05		C
ATOM	1618	N			335	69.588	58.506	29.491	1.00	24.43		N
		CA			335	70.181	57.256	29.964		24.60		C
ATOM	1619					70.774	57.420			25.20		C
MOTA	1620	С			335					26.11		. 0
MOTA	1621	0			335	70.484	56.635	32.271				C
MOTA	1622	CB			335	71.288	56.765	28.995				
MOTA	1623	CG1	VAL	A	335	71.986	55.527	29.564		25.97		C
MOTA	1624	CG2	VAL	Α	335	70.678	56.442	27.640		24.78		C
MOTA	1625	N	ILE	Α	336	71.600	58.448	31.533	1.00	25.74		N
MOTA	1626	CA	ILE	Α	336	72.238	58.713	32.815	1.00	26.05		C
ATOM	1627	C			336	71.213	58.842	33.945	1.00	27.20		C
MOTA	1628	ō			336	71.395	58.287	35.030	1.00	26.21		0
		CB			336	73.084	59.998	32.744		25.46		C
MOTA	1629					74.275	59.769	31.806		24.75		C
MOTA	1630		ILE							22.41		C
ATOM	1631		ILE			73.552	60.409	34.141				. c
MOTA	1632		ILE			75.078	61.022	31.519		26.47		
MOTA	1633	N	ASP	А	337	70.130	59.565	33.681		27.99		N
ATOM	1634	CA	ASP	A	337	69.090	59.769	34.686		28.97		C
MOTA	1635	C	ASP	Α	337	68.318	58.476	35.001		29.22		С
ATOM	1636	Ō			337	68.057	58.160	36.165	1.00	27.09		0
ATOM	1637	CB			337	68.110	60.845	34.209		31.92		С
MOTA	1638	CG			337	67.111	61.234	35.279		35.94		C
ATOM	1020	٠٠	rot.		J J /	07.111	U J	,				-

MOTA	1639	OD1	ASP	Α	337	66.026	61.755	34.937	1.00 39.65	0
ATOM	1640	OD2	ASP	Α	337	67.416	61.026	36.472	1.00 40.82	0
MOTA	1641	N	VAL	Α	338	67.950	57.739	33.956	1.00 27.65	N
MOTA	1642	CA	VAL	Α	338	67.205	56.502	34.133	1.00 26.39	C
MOTA	1643	C	VAL	Α	338	68.058	55.470	34.854	1.00 25.81	C
ATOM	1644	0	VAL	A	338	67.575	54.780	35.748	1.00 25.37	0
MOTA	1645	CB	VAL			66.720	55.930	32.771	1.00 24.93	C
ATOM	1646		VAL		•	66.113	54.545	32.971	1.00 23.01	
ATOM	1647		VAL			65.677	56.870	32.155	1.00 23.63	
MOTA	1648	N	VAL			69.323	55.375	34.460	1.00 25.47	
ATOM	1649	CA	VAL			70.252	54.440	35.075	1.00 25.33	
ATOM	1650	C	VAL			70.232	54.711	36.572	1.00 27.56	
		0	VAL			70.413	53.773	37.362	1.00 27.00	
MOTA	1651						54.500	34.383	1.00 23.02	
ATOM	1652	CB	VAL			71.633				
ATOM	1653		VAL			72.701	53.830	35.246	1.00 23.64	
ATOM	1654		VAL			71.549	53.809	33.031	1.00 22.84	
MOTA	1655	N	ALA			70.458	55.982	36.962	1.00 27.28	
ATOM	1656	CA	ALA			70.596	56.330	38.374	1.00 28.29	
MOTA	1657	C			340	69.360	55.861	39.141	1.00 29.41	
ATOM	1658	0			340	69.461	55.348	40.260	1.00 29.34	
MOTA	1659	CB	ALA			70.775	57.835	38.536	1.00 25.77	
MOTA	1660	N	GLU			68.192	56.031	38.531	1.00 28.19	
ATOM	1661	CA	GLU	Α	341	66.949	55.619	39.168	1.00 29.67	
MOTA	1662	C	GLU	А	341	66.878	54.093	39.245	1.00 28.17	
ATOM	1663	0	GLU	Α	341	66.419	53.543	40.236	1.00 27.43	
ATOM	1664	CB	GLU	Α	341	65.750	56.151	38.384	1.00 30.31	
ATOM	1665	CG	GLU	Α	341	64.433	56.116	39.153	1.00 33.93	
MOTA	1666	CD	GLU	Α	341	64.441	57.036	40.368	1.00 36.33	
ATOM	1667	OE1	GLU	Α	341	65.031	58.137	40.294	1.00 37.90	0
ATOM	1668	OE2	GLU	Α	341 .	63.843	56.668	41.395	1.00 37.92	2 0
MOTA	1669	N	ARG	Α	342	67.335	53.420	38.192	1.00 28.17	
ATOM	1670	CA	ARG	Α	342	67.328	51.959	38.140	1.00 27.23	
MOTA	1671	C	ARG	Α	342	68.220	51.382	39.241	1.00 26.35	S C
MOTA	1672	0	ARG	Α	342	67.861	50.394	39.875	1.00 27.18	0
ATOM	1673	CB	ARG	Α	342	67.799	51.481	36.756	1.00 26.16	c c
ATOM	1674	CG	ARG	Α	342	67.736	49.961	36.513	1.00 25.83	L C
MOTA	1675	CD	ARG	Α	342 -	68.988	49.223	37.006	1.00 22.94	L C
MOTA	1676	NE	ARG	Α	342	70.230	49.706	36.405	1.00 23.3	7 N
ATOM	1677	CZ			342	70.606	49.502	35.141	1.00 22.98	3 C
ATOM	1678	NH1			342	69.837	48.816	34.304	1.00 22.09	N N
ATOM	1679		ARG			71.771	49.977	34.713	1.00 22.35	5 N
ATOM	1680	N			343	69.372	52.005	39.472	1.00 26.04	
ATOM	1681	CA			343	70.288	51.542	40.510	1.00 27.90	
ATOM	1682	C			343	69.715	51.821	41.902	1.00 30.25	
ATOM	1683	0			343	69.891	51.030	42.827	1.00 31.34	
ATOM	1684	СВ			343	71.662	52.202	40.353	1.00 25.88	
ATOM	1685	CG			343	72.379	51.755	39.086	1.00 28.08	
ATOM	1686		ASN			72.029	50.729	38.494	1.00 26.63	
	1687		ASN			73.396	52.510	38.674	1.00 26.34	
ATOM	1688	N			344	69.017	52.941	42.043	1.00 31.3	
ATOM	1689	CA			344	68.392	53.296	43.308	1.00 34.03	
	1690	C			344	67.296	52.260	43.561	1.00 33.69	
ATOM ATOM	1691	0			344	67.151	51.736	44.668	1.00 34.4	
	1691	CB			344	67.791	54.705	43.209	1.00 34.4	
ATOM ATOM	1692	CG			344	67.791	55.221	44.467	1.00 30.2	
ATOM	1693	CD			344	66.596	56.654	44.257	1.00 46.73	
ATOM	1695	CE				65.820	57.178	45.469	1.00 49.4	
111011	1000	<u> </u>			J 1 1	00.020	5		1.00 40.40	

MOTA	1696	NZ	LYS	Α	344	66.664	57.318	46.702	1.00 53.65		N
ATOM	1697	N	TYR	Α	345	66.541	51.956	42.512	1.00 32.48		N
MOTA	1698	CA	TYR	A	345	65.463	50.979	42.590	1.00 32.33		С
ATOM	1699	С	TYR			66.008	49.599	42.989	1.00 32.68		C
ATOM	1700	0	TYR			65.413	48.901	43.811	1.00 32.28		0
MOTA	1701	CB	TYR			64.764	50.878	41.241	1.00 30.33		C
ATOM	1702	CG	TYR			63.474	50.092	41.273			С
ATOM	1702	CD1	TYR			62.291	50.685	41.702	1.00 32.27		C
		CD2	TYR			63.427	48.767	40.830	1.00 31.10		C
ATOM	1704					61.090	49,988	41.681	1.00 32.84		C
ATOM	1705	CE1	TYR				48.061	40.805	1.00 32.54		C
ATOM	1706	CE2	TYR			62.230		41.228	1.00 32.54		C
MOTA	1707	CZ	TYR			61.066	48.683		1.00 35.30		0
MOTA	1708	OH	TYR			59.869	48.022	41.152			N
MOTA	1709	N	PHE			67.133	49.211	42.396	1.00 32.82		
MOTA	1710	CA	PHE			67.759	47.928	42.703	1.00 34.48		C
MOTA	1711	C	PHE			68.103	47.840	44.193	1.00 35.77		C
ATOM	1712	0	PHE			67.859	46.827	44.843	1.00 34.19		0
MOTA	1713	CB	PHE	А	346	69.037	47.751	41.881	1.00 34.20		C
MOTA	1,714	.CG	PHE	Α	346	69.817	46.518	42.232	1.00 35.55		C
ATOM	1715	CD1	PHE	Α	346	69.302	45.254	41.964	1.00 34.50		С
MOTA	1716	CD2	PHE	А	346	71.060	46.620	42.850	1.00 37.04		C
ATOM	1717	CE1	PHE	Α	346	70.010	44.107	42.304	1.00 35.77		C
MOTA	1718	CE2	PHE	A	346	71.779	45.478	43.198	1.00 38.55		C
ATOM	1719	CZ	PHE	A	346	71.250	44.217	42.923	1.00 38.73		C
MOTA	1720	N	GLU	A	347	68.660	48.921	44.723	1.00 37.60		N
ATOM	1721	CA	GLU	A	347	69.054	48.986	46.122	1.00 40.87		С
MOTA	1722	С	GLU	A	347	67.875	48.954	47.091	1.00 40.71		С
MOTA	1723	0	GLU	А	347	68.014	48.483	48.218	1.00 41.55		0
MOTA	1724	CB	GLU	Α	347	69.887	50.247	46.361	1.00 42.18		С
MOTA	1725	CG	GLU	Α	347	71.112	50.334	45.461	1.00 49.56		С
MOTA	1726	CD	GLU	Α	347	72.249	49.423	45.901	1.00 54.08		C
ATOM	1727	OE1	GLU	Α	347	71.994	48.244	46.240	1.00 57.12		0
MOTA	1728	OE2	GLU	Α	347	73.412	49.887	45.899	1.00 57.88		0
ATOM	1729	N	GLU	A	348	66.717	49.446	46.656	1.00 39,71		N
ATOM	1730	CA	GLU	A	348	65.543	49.464	47.523	1.00 39.97	•	С
ATOM	1731	С	GLU	Α	348	64.782	48.149	47.503	1.00 38.48		C
MOTA	1732	0	GLU	Α	348	64.283	47.705	48.529	1.00 38.26		0
MOTA	1733	CB	GLU	Α	348	64.543	50.550	47.100	1.00 41.21		C
MOTA	1734,	CG	GLU	·A	348	65.120	51.879	46.664	1.00 44.97		C
MOTA	1735		GLU	Α	348	64.044	52.828	46.141	1.00 45.86		C
MOTA	1736		GLU	Α	348	63.112	52.360	45.454	1.00 46.60		0
MOTA	1737	OE2	GLU	A	348	64.135	54.043	46.405	1.00 48.18		0
MOTA	1738	N			349	64.696	47.536	46.327	1.00 37.21		N
MOTA	1739	CA	THR	A	349	63.922	46.314	46.146	1.00 35.37		· C
ATOM	1740	С	THR	Α	349	64.677	45.019	45.849	1.00 35.43		С
MOTA	1741	O.			349	64.093	43.943	45.910	1.00 36.36		0
MOTA	1742	CB			349	62.906	46.507	45.004	1.00 35.82		C
MOTA	1743	OG1	THR			63.613	46.564	43.755	1.00 33.52		0
MOTA	1744		THR			62.116	47.812	45.190	1.00 34.32		· C
ATOM	1745	N			350	65.957	45.114	45.513	1.00 35.89		N
MOTA	1746	CA			350	66.715	43.917	45.183	1.00 34.68		С
ATOM	1747	C			350	66.415	43.442	43.766	1.00 33.95		С
ATOM	1748	Ö			350	66.870	42.381	43.339	1.00 35.21		0
ATOM	1749	N			351	65.639	44.231	43.029	1.00 33.01		N
ATOM	1750	CA			351	65.283	43.885	41.654	1.00 30.90		С
ATOM	1751	C			351	66.124					C
ATOM	1752	0			351	66.117		40.699			0
		-									

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ATOM	1753	CB	ILE				63.795	44.197	41.356	1.00			С
MOTA	1754	CG1	ILE	Α	351		62.885	43.471	42.355	1.00	34.74		С
ATOM	1755	CG2	ILE	Α	351		63.455	43.779	39.930	1.00	32.48		С
ATOM	1756	CD1	ILE	Α	351		61.424	43.894	42.262	1.00	34.70		C
MOTA	1757	N	TYR	Α	352		66.842	44.005	39.785	1.00	28.99		N
ATOM	1758	CA	TYR				67.655	44.685	38.787	1.00	28.73		C
	1759	C	TYR				66.907	44.657	37.464	1.00			С
ATOM							66.651	43.588	36.921	1.00			Ō
ATOM	1760	0	TYR						38.593	1.00			C
ATOM	1761	CB	TYR				69.004	43.991					C
MOTA	1762	CG	TYR				69.899	44.726	37.617	1.00			C
ATOM	1763	CD1	TYR				70.688	45.799	38.038	1.00			
ATOM	1764	CD2	TYR				69.925	44.376	36.267	1.00			C
MOTA	1765	CE1	TYR	Α	352		71.481	46.504	37.139	1.00			C
MOTA	1766	CE2	TYR	А	352	•	70.715	45.076	35.358	1.00	26.68		С
ATOM	1767	CZ	TYR	А	352		71.492	46.138	35.804	1.00	24.57		C
ATOM	1768	OH	TYR	Α	352		72.302	46.809	34.923	1.00	26.41		0
ATOM	1769	N	ILE	А	353		66.554	45.831	36.948	1.00	28.02		N
ATOM	1770	CA	ILE				65.843	45.897	35.681	1.00	26.70		C
ATOM	1771	C	ILE				66.761	46.407	34.575	1.00	27.00		C
ATOM	1772	Ō	ILE				67.247	47.536	34.631	1.00	27.67		0
ATOM	1773	CB	ILE				64.620	46.826	35.780		28.56		С
			ILE				63.702	46.346	36.915		29.44		C
ATOM	1774						,		34.443		28.04		C
ATOM	1775		ILE				63.875	46.840			27.09		C
ATOM	1776		ILE				62.450	47.169	37.103				
MOTA	1777	N	PRO				67.020	45.574	33.556		26.94		N
MOTA	1778	CA	PRO				67.892	45.999	32.456		25.14		C
MOTA	1779	С	PRO	A	354		67.246	47.162	31.711		25.78		C
MOTA	1780	0	PRO	A	354		66.020	47.210	31.578		24.81		0
MOTA	1781	CB	PRO	Α	354		67.988	44.748	31.582		23.53		С
MOTA	1782	CG	PRO	Α	354	-	67.734	43.614	32.558	1.00	24.17	•	C
MOTA	1783	CD	PRO	Α	354		66.612	44.167	33.392	1.00	25.08		C
ATOM	1784	N	VAL	Α	355		68.061	48.106	31.242	1.00	25.52		N
ATOM	1785	CA	VAL				67.524	49.237	30.498	1.00	24.60		C
ATOM	1786	C	VAL				68.152	49.287	29.124	1.00	24.64		C
MOTA	1787	Ō			355		69.309	48.914	28.937	1.00	24.59		0
ATOM	1788	CB			355		67.727	50.596	31.233		24.72		C
ATOM	1789		VAL				66.987	50.566	32.560		23.24		С
			VAL				69.209	50.905	31.425		22.37		C
ATOM	1790						67.365	49.746	28.163		24.56		N
ATOM	1791	N			356				26.783		24.50		C
ATOM	1792	CA			356			49.819			24.85		C
MOTA	1793	C			356		67.869	51.245	26.263				
MOTA	1794	0			356		66.901		26.368		25.28		0
MOTA	1795	CB			356		66.816	49.018	25.919		24.42		C
MOTA	1796	SG			356		67.077		24.147		27.02		S
MOTA	1797	N	SER	Α	357		69.017		25.704		24.06		N
MOTA	1798	CA	SER	Α	357		69.172	52.944	25.123	1.00	24.90		C
MOTA	1799	C	SER	Α	357		68.681	52.774	23.694	1.00	24.81		С
MOTA	1800	0	SER	A	357		69.300	52.076	22.897	1.00	24.49		0
MOTA	1801	CB			357		70.629	53.394	25.110	1.00	23.83		С
ATOM	1802	OG			357		70.717	54.691	24.539	1.00	26.00		0
MOTA	1803	N			358		67.562	53.414	23.389		25.07		N
MOTA	1804	CA			358		66.927	53.308	22.085		26.86		C
ATOM	1805	C			358		67.067	54.547	21.200		26.28		C
							66.510	55.598	21.504		25.81		ō
ATOM	1806	O			358				22.309		26.49		C
ATOM	1807	CB			358		65.442				26.81		C
ATOM	1808	CG			358		64.672		21.021				0
ATOM	1809	OD1	ASP	A	358		65.293	52.598	19.949	1.00	28.14		

MOTA	1810	OD2	ASP	A	358	63.425	52.757	21.099	1.00 25.3	2	0
MOTA	1811	N	GLY	A	359	67.811	54.409	20.106	1.00 28.2	8	N
MOTA	1812	CA	GLY	A	359	67.975	55.509	19.174	1.00 30.2	0	С
ATOM	1813	C	GLY	A	359	69.098	56.486	19.460	1.00 33.1	1	C
MOTA	1814	0	GLY	Α	359	69.637	56.539	20.564	1.00 32.4	9	0
ATOM	1815	N	GLY	Α	360	69.456	57.260	18.442	1.00 34.0	1	N
MOTA	1816	CA	GLY	A	360	70.504	58.243	18.602	1.00 36.3	0	C
MOTA	1817	C	GLY	Α	360	71.916	57.755	18.357	1.00 37.1	6	C
MOTA	1818	0			360	72.849	58.538	18.482	1.00 39.1	8	0
MOTA	1819	N			361	72.096	56.481	18.021	1.00 38.4	7	N
ATOM	1820	CA	ILE	А	361	73.442	55.976	17.762	1.00 40.2	2	С
MOTA	1821	С	ILE	Α	361	73.856	56.399	16.359	1.00 42.5	1	C
MOTA	1822	0	ILE	Α	361	73.296	55.922	15.369	1.00 42.1	4	0
MOTA	1823	CB	ILE	A	361	73.527	54.430	17.848	1.00 40.0	3	С
MOTA	1824	CG1	ILE	А	361	73.133	53.945	19.247	1.00 38.7	0	C
MOTA	1825	CG2	ILE	Α	361	74.953	53.974	17.527	1.00 39.3	0	C
ATOM	1826	CD1	ILE			74.077	54.379	20.352	1.00 38.3	5	С
MOTA	1827	N	VAL	Α	362	74.835	57.297	16.284	1.00 44.1	3	N
ATOM	1828	CA	VAL	Α	362	75.326	57.799	15.007	1.00 45.1	8	С
ATOM	1829	C	VAL	А	362	76.688	57.200	14.659	1.00 46.1	8	C
ATOM	1830	0	VAL	A	362	76.943	56.875	13.498	1.00 47.5	4	0
ATOM	1831	CB	VAL	Α	362	75.437	59.336	15.030	1.00 46.1	1	C
ATOM	1832	CG1	VAL	Α	362	75.853	59.856	13.653	1.00 47.6	4	С
ATOM	1833	CG2	VAL	Α	362	74.099	59.940	15.440	1.00 47.3	3	C
ATOM	1834	N	TYR	А	363	77.552	57.052	15.665	1.00 44.6	3	N
MOTA	1835	CA	TYR	Α	363	78.889	56.482	15.473	1.00 42.5	2	C
ATOM	1836	C	TYR	Α	363	79.087	55.265	16.370	1.00 39.5	0	С
ATOM	1837	0	TYR	Α	363	78.395	55.109	17.373	1.00 38.8	0	0
MOTA	1838	CB	TYR	Α	363	79.960	57.519	15.803	1.00 44.7	2	C
ATOM	1839	CG	TYR	Α	363	79.838	58.794	15.010	1.00 48.9	1	C
MOTA	1840	CD1	TYR	Α	363	79.930	58.782	13.619	1.00 51.1	3	C
ATOM	1841	CD2	TYR	А	363	79.639	60.016	15.649	1.00 50.1	2	C
ATOM-	1842	CE1	TYR	Α	363	79.829	59.957	12.882	1.00 53.5	3	С
MOTA	1843	CE2	TYR			79.538	61.199	14.921	1.00 52.9		С
ATOM	1844	CZ			363	79.636	61.162		1.00 53.7		C
MOTA	1845	OH			363	79.567	62.330	12.813	1.00 56.3		0
ATOM	1846	N			364	80.040	54.409	16.024	1.00 37.7		N
ATOM	1847	CA			364	80.289	53.221	16.831	1.00 37.3		С
ATOM	1848	С			364	80.610	53.556	18.282	1.00 36.2		С
MOTA	1849	0			364	80.175	52.852		1.00 37.3		0
ATOM	1850	CB			364	81.441	52.389	16.259	1.00 39.5		C
MOTA	1851	CG			364	81.104	51.746	14.926	1.00 41.1		С
MOTA	1852		ASP			79.976	51.235	14.763	1.00 40.9		0
ATOM	1853		ASP			81.985	51.738	14.042	1.00 44.4		0
MOTA	1854	N			365	81.359	54.631	18.508	1.00 33.8		N
MOTA	1855	CA			365	81.733	54.989	19.870	1.00 33.0		C
ATOM	1856	C			365	80.544	55.418	20.733	1.00 31.6		C
MOTA	1857	0			365	80.646	55.456	21.955	1.00 30.0		0
ATOM	1858	CB			365	82.828	56.066	19.859	1.00 31.2		C
ATOM	1859	CG			365	82.342	57.493	19.813	1.00 34.9		C
ATOM	1860		TYR			82.131	58.216	20.987	1.00 35.2		C
ATOM	1861		TYR			82.136	58.140	18.595	1.00 36.0		C
ATOM	1862		TYR			81.735	59.549	20.948	1.00 37.4		C
MOTA	1863	CE2			365	81.738	59.476	18.545	1.00 38.4		C
ATOM	1864	CZ			365	81.543	60.173	19.724	1.00 38.6		C
MOTA	1865	OH			365	81.174	61.500	19.676	1.00 43.0		O N
MOTA	1866	N	uis	А	366	79.420	55.737	20.098	1.00 31.3	,	N

MOTA	1867	CA	HIS	A	366	78.231	56.110	20.850	1.00 30.85	С
MOTA	1868	C	HIS	A	366	77.743	54.859	21.571	1.00 28.97	C
MOTA	1869	0	HIS	A	366	77.130	54.947	22.630	1.00 28.47	0
MOTA	1870	CB	HIS	A	366	77.125	56.635	19.926	1.00 31.13	C
MOTA	1871	CG	HIS	A	366	77.373	58.016	19.406	1.00 31.77	C
MOTA	1872	ND1	HIS	Α	366	78.311	58.862	19.957	1.00 33.13	N
ATOM	1873	CD2	HIS	A	366	76.765	58.719	18.422	1.00 31.89	С
MOTA	1874	CE1	HIS	Α	366	78.267	60.028	19.339	1.00 31.00	С
MOTA	1875	NE2	HIS	Α	366	77.337	59.968	18.405	1.00 32.26	N
MOTA	1876	N	MET	A	367	78.017	53.697	20.979	1.00 27.68	N
MOTA	1877	CA	MET	A	367	77.633	52.419	21.580	1.00 28.37	C
ATOM	1878	С	MET	A	367	78.372	52.283	22.909	1.00 26.83	C
ATOM	1879	0	MET	A	367	77.774	51.998	23.938	1.00 27.33	0
ATOM	1880	CB	MET	A	367	78.027	51.240	20.678	1.00 26.41	C
ATOM	1881	CG	MET	A	367	77.301	51.164	19.333	1.00 29.28	C
ATOM	1882	SD	MET	Α	367	77.864	49.737	18.350	1.00 31.67	s
MOTA	1883	CE	MET	A	367	76.804	49.861	16.903	1.00 31.17	,C
ATOM	1884	N	THR	A	368	79.686	52.485	22.868	1.00 27.26	N
MOTA	1885	CA	THR	A	368	80.519	52.393	24.062	1.00 27.02	C
ATOM	1886	C	THR	A	368	80.035	53.402	25.106	1.00 26.24	С
MOTA	1887	0	THR	A	368	79.960	53.092	26.288	1.00 26.81	0
ATOM	1888	CB	THR	A	368	81.998	52.667	23.713	1.00 27.29	C
ATOM	1889	OG1	THR	A	368	82.350	51.907	22.548	1.00 28.57	0
MOTA	1890	CG2	THR	Α	368	82.912	52.252	24.861	1.00 26.87	С
MOTA	1891	N	LEU	A	369	79.701	54.610	24.664	1.00 25.92	N
ATOM	1892	CA	LEU	A	369	79.205	55.636	25.578	1.00 27.25	C
MOTA	1893	C	LEU	Α	369	77.913	55.206	26.263	1.00 25.90	С
ATOM	1894	0	LEU	А	369	77.805	55.280	27.483	1.00 26.13	0
MOTA	1895	CB	LEU	A	369	78.956	56.949	24.835	1.00 27.34	C
MOTA	1896	CG	LEU	A	369	80.177	57.813	24.525	1.00 30.74	С
MOTA	1897	CD1	LEU	Α	369	79.731	59.030	23.718	1.00 30.74	C
MOTA	1898	CD2	LEU	Α	369	80.855	58.244	25.823	1.00 27.53	С
MOTA	1899	N	ALA	А	370	76.946	54.755	25.464	1.00 25.24	N
MOTA	1900	CA	ALA	A	370	75.644	54.313	25.966	1.00 25.58	С
MOTA	1901	С	ALA	Α	370	75.804	53.233	27.037	1.00 23.76	С
MOTA	1902	Ο.	ALA	A	370	75.192	53.294	28.099	1.00 24.01	0
ATOM	1903	CB	ALA	Α	370	74.792	53.787	24.809	1.00 20.78	C
MOTA	1904	N	LEU	Α	371	76.638	52.248	26.745	1.00 24.06	N
MOTA	1905	CA	LEU	A	371	76.892	51.162	27.677	1.00 24.06	C
MOTA	1906	C	LEU	Α	371	77.599	51.698	28.926	1.00 24.64	С
ATOM	1907	0	LEU	А	371	77.223	51.360	30.042	1.00 24.05	0
MOTA	1908	CB	LEU	Α	371 ·	77.750	50.086	26.990	1.00 22.32	C
MOTA	1909	CG	LEU	Α	371	77.084	49.415	25.772	1.00 25.62	C
MOTA	1910	CD1	LEU	A	371	78.104	48.572	25.004	1.00 24.75	С
ATOM	1911	CD2	LEU	A	371	75.909	48.553	26.227	1.00 23.36	C
MOTA	1912	N	ALA	Α	372	78.607	52.549	28.732	1.00 23.99	N
MOTA	1913	CA	ALA	Α	372	79.367	53.109	29.844	1.00 24.54	С
MOTA	1914	C	ALA			78.484	53.911	30.774	1.00 26.37	C
ATOM	1915	0	ALA	A	372	78.699	53.920	31.984	1.00 26.64	0
MOTA	1916	CB	ALA			80.505	53.989	29.329	1.00 23.23	. C
MOTA	1917	N	MET	A	373	77.496	54.598	30.207	1.00 26.85	N
MOTA	1918	CA	MET			76.591	55.395	31.017	1.00 26.45	C
MOTA	1919	С	MET			75.617	54.514	31.795	1.00 25.55	С
MOTA	1920 ·	0	MET			74.883	55.009	32.634	1.00 26.24	0
MOTA	1921	CB	MET			75.834	56.402	30.145	1.00 25.35	C
ATOM	1922	CG			373	76.704	57.547	29.626	1.00 27.17	C
MOTA	1923	SD	MET	A	373	75.865	58.517	28.344	1.00 27.74	S

ATOM	1924	CE	MET	A	373	77.157	59.681	27.884	1.00 2	6.78	C
ATOM	1925	N	GLY	A	374	75.603	53.212	31.518	1.00 2	5.87	N
MOTA	1926	CA	GLY	Α	374	74.725	52.327	32.269	1.00 2	4.01	С
MOTA	1927	C	GLY	A	374 .	73.710	51.500	31.506	1.00 2	4.90	С
MOTA	1928	0	GLY	A	374	73.120	50.581	32.073	1.00 2	6.82	0
MOTA	1929	N	ALA	A	375	73.472	51.818	30.241	1.00 2	3.59	N
ATOM	1930	CA	ALA	A	375	72.521	51.035	29.468	1.00 2	4.75	С
MOTA	1931	С	ALA	Α	375	73.061	49.611	29.345	1.00 2	5.43	С
MOTA	1932	0	ALA			74.255	49.411	29.116	1.00 2		0
ATOM	1933	CB	ΆLΑ			72.325	51.644	28.085	1.00 2		С
MOTA	1934	N	ASP			72.182	48.627	29.506	1.00 2		N
ATOM	1935	CA	ASP			72.571	47.221	29.406	1.00 2		C
ATOM	1936	C	ASP			72.671	46.809	27.945	1.00 2		С
MOTA	1937	0	ASP			73.531	46.017	27.573	1.00 2		0
ATOM	1938	CB	ASP			71.559	46.355	30.147	1.00 2		C
MOTA	1939	CG			376	71.472	46.713	31.616	1.00 2		С
ATOM	1940		ASP			72.272	46.174	32.413	1.00 2		0
ATOM	1941		ASP			70.616	47.549	31.971	1.00 2		0
MOTA	1942	N			377	71.779	47.339	27.117	1.00 2		N
MOTA	1943	CA			377	71.834		25.695	1.00 2		C
MOTA	1944	C			377	71.331	48.236	24.876	1.00 2		C
MOTA	1945	0			377	70.791	49.205	25.416	1.00 2		0
ATOM	1946	CB			377	71.108	45.742	25.327	1.00 2		C
ATOM	1947	CG			377	69.704	45.638	25.836	1.00 2		C
MOTA	1948		PHE			69.451	45.223	27.141	1.00 2		C
MOTA	1949		PHE			68.626	45.898	24.992	1.00 2		C
ATOM	1950		PHE			68.137	45.064	27.597	1.00 2		C
ATOM	1951		PHE			67.316	45.742	25.438	1.00 2		C
ATOM	1952	CZ			377	67.072	45.323	26.741	1.00 2		C
MOTA MOTA	1953 1954	N CA			378 378	71.526	48.150	23.567	1.00 2		N C
ATOM	1955	CA			378	71.188 70.242	49.241 48.824	22.669	1.00 2		C
ATOM	1956	0			378	70.242	47.774	20.947	1.00 2		0
ATOM	1957	CB			378	72.497	49.788	22.032	1.00 2		C
ATOM	1958	CG1			378	73.491	50.146	23.137	1.00 2		C
ATOM	1959		ILE			72.217	51.011	21.159	1.00 2		C
ATOM	1960		ILE			74.915	50.248	22.644	1.00 2		C
ATOM	1961	N	MET			69.226	49.641	21,301	1.00 2		N
ATOM	1962	CA			379	68.293	49.346	20.217	1.00 2		C
ATOM	1963	C.			379	68.654	50.271	19.054	1.00 2		C
ATOM	1964	Ō			379	68.784	51.478		1.00 2		ō
ATOM	1965	CB	MET			66.838	49.581	20.645	1.00 2		C
ATOM	1966	CG	MET			65.844	49.295		1.00 2		Ċ
ATOM	1967	SD	MET			64.114	49.244	20.007	1.00 2		s
ATOM	1968	CE			379	63.985	47.548	20.606	1.00 2		С
MOTA	1969	N			380	68.829	49.701	17.868	1.00 2		N
MOTA	1970	CA			380	69.181	50.503	16.706	1.00 2		С
MOTA	1971	С			380	68.279	50.225	15.516	1.00 2		C
MOTA	1972	0	LEU			67.880	49.086	15.275	1.00 2		0
ATOM	1973	CB			380	70.642	50.258	16.301	1.00 2	9.79	C
MOTA	1974	CG	LEU	A	380	71.722	50.470	17.368	1.00 3	0.01	С
MOTA	1975	CD1	LEU			71.783	49.227	18.259	1.00 3		С
MOTA	1976		LEU			73.079	50.693	16.714	1.00 3	0.65	С
MOTA	1977	N	GLY	A	381	67.960	51.283	14.780	1.00 3	0.37	N
MOTA	1978	CA	GLY	A	381	67.122	51.155	13.602	1.00 3	1.25	C
MOTA	1979	C	\mathtt{GLY}	A	381	67.941	51.401	12.348	1.00 3	0.92	С
MOTA	1980	0	\mathtt{GLY}	A	381	68.210	50.485	11.581	1.00 3	0.18	0

MOTA	1981	N	ARG	Α	382	68.351	52.646	12.147	1.00 3		N
ATOM	1982	CA	ARG	Α	382	69.142	53.014	10.977	1.00 3	6.36	С
ATOM	1983	С	ARG	Α	382	70.371	52.125	10.772	1.00 3	6.33	С
ATOM	1984	0	ARG			70.645	51.681	9.656	1.00 3	5.82	0
ATOM	1985	СВ	ARG			69.585	54.472	11.084	1.00 3	8.87	C
		CG	ARG			70.584	54.858	10.023	1.00 4		C
ATOM	1986					71.228	56.211	10.282	1.00 5		C
MOTA	1987	CD	ARG					9.470	1.00 5		N
ATOM	1988	NE	ARG			72.434	56.333		1.00 5		C
MOTA	1989	CZ	ARG			73.548	55.638	9.685			
MOTA	1990		ARG			73.614	54.780	10.700	1.00 5		N
MOTA	1991	NH2	ARG	A	382	74.582	55.774	8.863	1.00 5		N
MOTA	1992	N	TYR	Α	383	71.109	51.877	11.851	1.00 3		N
MOTA	1993	CA	TYR	Α	383	72.311	51.044	11.808	1.00 3		C
ATOM	1994	C	TYR	Α	383	72.059	49.714	11.093	1.00 3	2.20	С
ATOM	1995	0	TYR	Α	383	72.818	49.323	10.209	1.00 3	2.03	0
ATOM	1996	CB	TYR			72.808	50.781	13.237	1.00 3	1.93	C
ATOM	1997	CG	TYR			74.023	49.884	13.333	1.00 3	0.42	C
MOTA	1998	CD1	TYR			75.316	50.413	13.303	1.00 3		C
		CD2				73.879	48.501	13.445	1.00 2		 С
ATOM	1999		TYR			76.431	49.586	13.384	1.00 2		Ċ
MOTA	2000		TYR					13.527	1.00 2		Ċ
MOTA	2001	CE2	TYR			74.983	47.665		1.00 2		C
MOTA	2002	CZ	TYR			76.254	48.210	13.495			0
MOTA	2003	OH	TYR			77.342	47.373	13.556	1.00 2		
MOTA	2004	N	PHE	Α	384	70.988	49.029	11.477	1.00 3		N
MOTA	2005	CA	PHE	Α	384	70.635	47.741	10.884	1.00 3		C
ATOM	2006	С	PHE	Α	384	69.907	47.827	9.533	1.00 3		C
MOTA	2007	0	PHE	Α	384	69.951	46.886	8.744	1.00 3		0
ATOM	2008	CB	PHE	Α	384	69.773	46.939	11.862	1.00 3	0.96	С
MOTA	2009	CG	PHE	Α	384	70.526	46.421	13.063	1.00 3	2.53	C
MOTA	2010		PHE			71.443	45.375	12.931	1.00 2	9.92	C
MOTA	2011		PHE			70.301	46.963	14.330	1.00 2	28.33	C
ATOM	2012		PHE			72.123	44.874	14.045	1.00 3	0.70	С
ATOM	2012		PHE			70.971	46.471	15.444	1.00 3		С
		CZ			384	71.886	45.421	15.303	1.00 2		С
MOTA	2014				385	69.234	48.943	9.269	1.00 3		N
ATOM	2015	N					49.104	8.010	1.00 3		C
ATOM	2016	CA			385	68.504			1.00 3		Ċ
MOTA	2017	С			385	69.441	49.035	6.805			0
MOTA	2018	0			385	69.051	48.586	5.731	1.00 3		 C
MOTA	2019	CB			385		50.429	8.009	1.00 3		
MOTA	2020	N			386		49.475				N
MOTA	2021	CA	ARG	A	386	71.701	49.491	5.958	1.00 3		C
MOTA	2022	C	ARG	Α	386	72.150	48.109	5.488	1.00 4		C
ATOM	2023	0	ARG	Α	386	72.819	47.989	4.457	1.00 3		0
ATOM	2024	CB	ARG	A	386	72.945	50.232	6.449	1.00 4		С
MOTA	2025	CG	ARG	A	386	72.755	51.685	6.835	1.00 4	13.04	C
ATOM	2026	CD	ARG	A	386	74.036	52.170	7.499	1.00 4	45.06	C
ATOM	2027	NE			386	74.404	51.264	8.585	1.00 4	46.41	N
MOTA	2028	CZ			386	75.644	51.055	9.015	1.00 4	45.80	C
ATOM	2029		ARG			76.667		8.455	1.00 4		N
	2030		ARG			75.860		9.996	1.00		N
ATOM					387	71.798		6.238	1.00		N
ATOM	2031	N						5.883	1.00		C
ATOM	2032	CA			387	72.229			1.00		C
MOTA	2033	C			387	71.346		4.892	1.00		0
ATOM	2034	0			387	70.143		4.769			C
MOTA	2035	CB			387	72.417		7.149			
MOTA	2036	CG			387	73.319		8.183			. C
MOTA	2037	CD1	PHE	A	387	74.411	46.283	7.801	1.00	39.37	C

ATOM	2038	CD2	PHE	A	387	73.084	45.308	9.544	1.00 39.37	С
MOTA	2039	CEl	PHE	Α	387	75.255	46.855	8.755	1.00 40.23	С
ATOM	2040	CE2	PHE	А	387	73.921	45.872	10.510	1.00 38.11	C
ATOM	2041	CZ			387	75.009	46.648	10.117	1.00 39.23	C
MOTA	2042	N	GLU	Α	388	71.985	44.040	4.190	1.00 42.30	N
ATOM	2043	CA	GLU			71.340		3.200	1.00 42.95	С
ATOM	2044	C	GLU			70.103		3.784	1.00 41.98	C
ATOM	2045	Ō	GLU			69.080		3.108	1.00 41.50	0
ATOM	2046	СВ	GLU			72.331	•	2.740	1.00 44.78	Ċ
ATOM	2047	CG	GLU			71.786		1.749	1.00 48.50	c
ATOM	2048	CD	GLU			71.457		0.400	1.00 51.34	C
ATOM	2049		GLU			72.306		-0.130	1.00 52.78	0
ATOM	2050		GLU			70.359		-0.134	1.00 53.13	0
ATOM	2051	N			389	70.333		5.049	1.00 40.73	N
ATOM	2052	CA			389	69.107		5.722	1.00 40.73	C
ATOM	2053	C	GLU					6.125	1.00 38.63	C
			GLU			67.884				0
ATOM	2054	O				66.879		6.541	1.00 38.65	
ATOM	2055	CB			389	69.648		6.937	1.00 39.65	C
ATOM	2056		GLU			70.631		6.567	1.00 39.31	C
ATOM	2057	CD			389	72.088		6.699	1.00 39.13	. C
ATOM	2058		GLU			72.409		6.511	1.00 37.80	0
MOTA	2059	OE2	GLU			72.924		6.982	1.00 38.72	0
MOTA	2060	N			390	67.951		6.020	1.00 38.90	N
ATOM	2061	CA			390	66.783		6.362	1.00 42.49	C
MOTA	2062	С			390	65.734		5.276	1.00 44.51	С
MOTA	2063	0			390	66.069		4.092	1.00 44.30	0
MOTA	2064	CB			390	67.130		6.393	1.00 41.33	C
MOTA	2065	OG	SER	A	390	67.521	46.348	5.116	1.00 46.43	0
MOTA	2066	N			391	64.454	43.985	5.669	1.00 45.30	N
MOTA	2067	CA	PRO	Α	391	63.317	43.691	4.785	1.00 47.36	C
MOTA	2068	C	PRO	Α	391	62.956	44.730	3.725	1.00 48.75	C
MOTA	2069	0	PRO	А	391	61.909	44.625	3.089	1.00 50.35	0
MOTA	2070	CB	PRO	Α	391	62.176	43.478	5.775	1.00 46.19	C
ATOM	2071	CG	PRO	Α	391	62.473	44.525	6.804	1.00 44.91	C
ATOM	2072	CD	PRO	Α	391	63.975	44.374	7.010	1.00 44.19	C
MOTA	2073	N	THR	Α	392	63.806	45.727	3.529	1.00 49.99	N
MOTA	2074	CA	THR	Α	392	63.507	46.755	2.549	1.00 51.23	С
ATOM	2075	C	THR	A	392	64.213	46.535	1.217	1.00 53.82	С
MOTA	2076	0	THR	·A	392	65077	45.665	1.083	1.00 54.85	 . 0
MOTA	2077	CB	THR	Α	392	63.863	48.152	3.084	1.00 49.99	С
ATOM	2078	OG1	THR	А	392	65.261	48.209	3.375	1.00 50.17	0
MOTA	2079	CG2	THR	A	392	63.070	48.450	4.351	1.00 49.74	C
MOTA	2080	N	ARG	Α	393	63.835		0.230	1.00 55.66	N
ATOM	2081	CA			393	64.407		-1.098	1.00 58.14	С
MOTA	2082	С			393	65.744		-1.238	1.00 58.48	C
MOTA	2083	0			393	65.950		-0.709	1.00 57.12	0
MOTA	2084	CB	ARG	А	393	63.419		-2.134	1.00 59.64	С
ATOM	2085	CG			393	62.178		-2.315	1.00 62.55	C
ATOM	2086	CD			393	61.092		-3.073	1.00 64.17	c
ATOM	2087	NE			393	61.646		-4.210	1.00 65.75	N
ATOM	2088	CZ			393	61.462		-4.423	1.00 67.27	C
ATOM	2089		ARG			60.732		-3.576	1.00 66.89	N
ATOM	2090		ARG			62.024		-5.472	1.00 68.47	N
MOTA	2090	N			394	66.650		-1.957	1.00 59.95	N
ATOM	2091	CA			394	67.979		-2.217	1.00 53.33	C
ATOM	2092	CA			394	67.835	•		1.00 61.71	C
								-3.479		
MOTA	2094	0	TX2	А	394	67.576	48.116	-4.555	1.00 64.78	0

ATOM	2095	CB	LYS			68.953	46.652	-2.456	1.00 59.47	C
MOTA	2096	CG	LYS	Α	394	70.408	47.017	-2.271	1.00 57.65	C
MOTA	2097	CD	LYS	Α	394	71.316	45.886	-2.715	1.00 56.24	С
MOTA	2098	CE	LYS	А	394	71.039	44.606	-1.958	1.00 54.65	C
MOTA	2099	NZ	LYS	A	394	71.894	43.500	-2.462	1.00 53.21	N
ATOM	2100	N	VAL	A	395	67.994	49.959	-3.343	1.00 66.61	N
ATOM	2101	CA	VAL	A	395	67.840	50.863	-4.474	1.00 69.32	C
ATOM	2102	C	VAL	А	395	69.118	51.577	-4.896	1.00 71.12	С
MOTA	2103	0	VAL	A	395	69.663	52.384	-4.145	1.00 71.80	0
MOTA	2104	CB	VAL	A	395	66.775	51.935	-4.168	1.00.69.81	C
ATOM	2105	CG1	VAL	A	395	66.653	52.901	-5.338	1.00 71.62	C
ATOM	2106	CG2	VAL	A	395	65.438	51.270	-3.884	1.00 70.98	С
ATOM	2107	N			396	69.581	51.287	-6.109	1.00 73.05	N
ATOM	2108	CA			396 ·	70.783	51.921	-6.644	1.00 74.05	С
MOTA	2109	С	THR			70.409	53.303	-7.163	1.00 74.87	C
ATOM	2110	0	THR			69.793	53.428	-8.222	1.00 75.03	0
ATOM	2111	СВ	THR			71.381	51.106	-7.804	1.00 74.00	c
ATOM	2112	OG1				71.715	49.791	-7.343	1.00 74.43	0
ATOM	2113	CG2	THR			72.638	51.781	-8.336	1.00 74.35	c
MOTA	2114		ILE			70.784	54.335	-6.415	1.00 75.83	N
MOTA	2115	CA			397	70.704	55.710	-6.788	1.00 76.89	C
ATOM	2116	C			397	71.681	56.521	-7.251	1.00 70.03	C
ATOM	2117	0			397	72.537	56.897	-6.449	1.00 77.33	
ATOM									1.00 77.38	0
	2118	CB			397	69.817	56.466	-5.612		
MOTA	2119	CG1				68.525	55.761	-5.196	1.00 77.37	C
ATOM	2120	CG2	ILE			69.538	57.911	-6.010	1.00 76.96	C
ATOM	2121		ILE			67.820	56.415	-4.025	1.00 78.15	C
ATOM	2122	N	ASN			71.736	56.793	-8.551	1.00 78.03	N
ATOM	2123	CA	ASN			72.814	57.583		1.00 77.85	C
ATOM	2124	C	ASN			74.200	57.051	-8.758	1.00 76.64	C
ATOM	2125	0	ASN			75.036	57.787	-8.229	1.00 76.51	0
MOTA	2126	CB	ASN			72.667	59.042	-8.679	1.00 79.57	C
ATOM	2127	CG	ASN			73.387	60.019	-9.595	1.00 82.07	C
ATOM	2128		ASN			74.617	60.007	-9.700	1.00 83.51	0
MOTA	2129	ND2	ASN	А	398	72.618	60.874	-10.266	1.00 82.25	N
MOTA	2130	N			399	74.434	55.768	-9.026	1.00 75.00	N
MOTA	2131	CA	GLY	A	399	75.724	55.165	-8.730	1.00 72.65	C
MOTA	2132	C	GLY	A	399	75.916	54.587	-7.336	1.00 71.38	С
MOTA	2133	0	GLY	Α	399	76.745	53.695	-7.143	1.00 71.58	0
MOTA	2134	.N	SER	Α	400	75.163	55.087	-6.361	1.00 69.39	N
MOTA	2135	CA	SER	Α	400	75.283	54.609	-4.985	1.00 66.71	С
MOTA	2136	C	SER	Α	400	74.121	53.723	-4.565	1.00 64.95	С
MOTA	2137	0	SER	Α	400	72.958	54.084	-4.734	1.00 65.32	0
ATOM	2138	CB	SER	Α	400	75.381	55.794	-4.023	1.00 66.11	C
MOTA	2139	OG	SER	Α	400	76.546	56.557	-4.273	1.00 66.69	0
MOTA	2140	N	VAL	A	401	74.440	52.561	-4.011	1.00 62.49	N
MOTA	2141	CA	VAL	Α	401	73.412	51.639	-3.557	1.00 60.52	C
MOTA	2142	C	VAL	Α	401	72.905	52.092	-2.190	1.00 60.36	C
MOTA	2143	0	VAL	Α	401	73.689	52.313	-1.261	1.00 60.61	0
ATOM	2144	CB	VAL			73.960	50.203	-3.453	1.00 59.89	C
ATOM	2145		VAL			72.869	49.261	-2.978	1.00 58.28	. С
ATOM	2146		VAL			74.496	49.758	-4.805	1.00 59.96	C
ATOM	2147	N			402	71.588	52.237		1.00 58.65	. N
ATOM	2148	CA	MET			70.957	52.672	-0.841	1.00 56.16	Ċ
ATOM	2149	C	MET			69.885	51.671	-0.435	1.00 54.18	C
ATOM	2150	0	MET			69.568	50.747	-1.186	1.00 53.12	0
ATOM	2151	CB	MET			70.297	54.038	-1.038	1.00 58.26	c
				- •			52.050	2.050	50.20	_

ATOM	2152	CG	MET	A	402	71.168	55.081	-1.713	1.00	59.17		C
ATOM	2153	SD	MET	A	402	72.561	55.584	-0.705	1.00	63.98		S
MOTA	2154	CE	MET	Α	402	71.781	56.836	0.332	1.00	60.67		C
ATOM	2155	N	LYS	A	403	69.340	51.856	0.764	1.00	51.25		N
ATOM	2156	CA	LYS			68.267	51.007	1.267	1.00	48.15		C
ATOM	2157	C	LYS	A	403	67.185	51.913	1.828	1.00	47.01		C
MOTA	2158	0	LYS			67.473	52.981	2.369	1.00	46.14		0
ATOM	2159	CB	LYS			68.760	50.049	2.357	1.00	47.38		C
MOTA	2160	CG	LYS			69.675	48.948	1.850		46.96		С
ATOM	2161	CD	LYS			69.389	47.602	2.514	1.00	46.69		C
ATOM	2162	CE	LYS			68.052	47.027	2.054		45.74		C
ATOM	2163	NZ	LYS			67.823	45.633	2.534		43.06		N
ATOM	2164	N	GLU			65.937	51.491	1.683		46.11		N
ATOM	2165	CA	GLU			64.817	52.276	2.171		46.13		С
ATOM	2166	С	GLU			64.767	52.246	3.689		44.64		C
ATOM	2167	0	GLU			65.107	51.243	4.316		43.82		0
MOTA	2168	CB	GLU			63.506	51.725	1.616		47.95		C
MOTA	2169	CG			404	63.453	51.663	0.101		52.21	,	C
MOTA	2170	CD	GLU			62.145	51.099	-0.405		53.46		C
MOTA	2171	OE1	GLU			61.875	49.900	-0.160		54.61		0
MOTA	2172	OE2	GLU			61.386	51.860	-1.042	1.00	54.88		0
MOTA	2173	Ν .	TYR			64.336	53.354	4.272	1.00	43.31		N
MOTA	2174	CA	TYR	Α	405	64.228	53.454	5.714	1.00	42.00		С
MOTA	2175	C			405	63.190	54.501	6.056	1.00	40.73		C
MOTA	2176	0	TYR	Α	405	63.323	55.662	5.688	1.00	41.74		0
ATOM	2177	CB	TYR	A	405	65.577	53.837	6.328	1.00	41.52		C
MOTA	2178	CG	TYR	Α	405	65.571	53.885	7.839	1.00	40.73		C
MOTA	2179	CD1	TYR	А	405	65.154	52.787	8.588	1.00	39.95		С
MOTA	2180	CD2	TYR	Α	405	66.002	55.020	8.521	1.00	40.92		C
MOTA	2181	CE1	TYR	Α	405	65.167	52.817	9.983	1.00	40.74		C
MOTA	2182	CE2	TYR	Α	405	66.019	55.061	9.913	1.00	40.89		C
MOTA	2183	CZ	TYR	Α	`405	65.599	53.957	10.637	1.00	40.10		C
MOTA	2184	OH	TYR	Α	405	65.596	54.003	12.011	1.00	39.70		0
MOTA	2185	N	TRP	A	406	62.150	54.082	6.760	1.00	39.11		N
MOTA	2186	CA	TRP	Α	406	61.091	54.993	7.153	1.00	37.83		C
MOTA	2187	С	TRP	Α	406	60.708	54.695	8.594	1.00	36.75		C
MOTA	2188	0	TRP	Α	406	60.862	53.566	9.057	1.00	36.18		0
ATOM	2189	CB	TRP	A	406	59.887	54.829	6.209	1.00	34.87		С
MOTA	2190	CG	TRP	Α	406	59.258	53.464	6.225	1.00.	32.13		C
MOTA	2191	CD1	TRP	Α	406	58.274	53.030	7.061	1.00	31.21		C
MOTA	·2192 ·	CD2	TRP	Α	406	59.574	52.357	5.371	1.00	31.79		С
MOTA	2193	NE1	TRP	Α	406	57.954	51.729	6.784	1.00	31.89	•	N
MOTA	2194	CE2	TRP	Α	406	58.736	51.287	5.752	1.00	31.65		C
MOTA	2195	CE3	TRP	A	406	60.483	52.165	4.322	1.00	32.48		C
MOTA	2196	CZ2	TRP	Α	406	58.776	50.034	5.119	1.00	32.31		C
ATOM	2197	CZ3	TRP	Α	406	60.524	50.915	3.690	1.00	33.57		C
MOTA	2198	CH2	TRP	Α	406	59.674	49.869	4.094	1.00	32.43		С
MOTA	2199	N	GLY	Α	407	60.229	55.717	9.298	1.00	37.66		N
MOTA	2200	CA	GLY	Α	407	59.835	55.554	10.685	1.00	38.09		C
ATOM	2201	C	GLY	А	407	58.446	54.963	10.858	1.00	39.18		С
MOTA	2202	0	GLY	Α	407	57.629	54.993	9.939	1.00	38.93		0
MOTA	2203	N	GLU	Α	408	58.183	54.419	12.042		39.46		N
ATOM	2204	CA			408	56.888	53.822	12.350	1.00	40.78		C
MOTA	2205	C			408	55.792	54.880	12.425		42.44		С
MOTA	2206	0			408	54.607	54.563	12.370		43.17		0
MOTA	2207	CB			408	56.963	53.062	13.674		39.22		C
ATOM	2208	CG	GLU	A	408	57.763	51.777	13.589		37.81		C

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MOTA	2209	CD	GLU			57.106	50.743	12.681	1.00 3			C
MOTA	2210		GLU			56.007	50.266	13.022	1.00 3			0
MOTA	2211	OE2	GLU	A	408	57.685	50.408	11.628	1.00 3			0
MOTA	2212	N	GLY			56.200	56.139	12.543	1.00 4			N
MOTA	2213	CA	GLY	A	409	55.242	57.227	12.623	1.00 4			C
MOTA	2214	C	GLY	Α	409	54.866	57.805	11.269	1.00 4			C
ATOM	2215	0	GLY	А	409	53.909 _.	58.566	11.166	1.00 4			0
MOTA	2216	N	SER	A	410	55.611	57.450	10.227	1.00 4			N
MOTA	2217	CA	SER	Α	410	55.316	57.956	8.893	1.00 9			С
ATOM	2218	C	SER	Α	410	54.028	57.319	8.381	1.00 5			C
ATOM	2219	0	SER	Α	410	53.676	56.205	8.777	1.00			0
ATOM	2220	CB	SER	Α	410	56.465	57.646	7.928	1.00			С
ATOM	2221	OG	SER	Α	410	56.489	56.273	7.580	1.00			0
MOTA	2222	N	SER	Α	411	53.328	58.033	7.503	1.00	55.87		N
MOTA	2223	CA	SER	A.	411	52.074	57.547	6.937	1.00	58.48		С
ATOM	2224	C	SER	Α	411	52.303	56.253	6.170	1.00			С
ATOM	2225	0	SER	A	411	51.425	55.393	6.100	1.00	59.90		0
ATOM	2226	CB '	SER	A	411	51.481	58.605	6.006	1.00	59.49		С
ATOM	2227	OG	SER	Α	411	52.433	59.025	5.042	1.00	60.32		0
ATOM	2228	N	ARG			53.498	56.122	5.605	1.00	61.10		N
ATOM	2229	CA	ARG			53.867	54.939	4.841	1.00	62.63		С
ATOM	2230	С	ARG	Α	412	53.824	53.667	5.686	1.00	64.23		C
ATOM	2231	0	ARG			54.057	52.572	. 5.177	1.00	63.68		0
ATOM	2232	СВ	ARG			55.273	55.114	4.254	1.00	60.98		C
ATOM	2233	CG	ARG			55.772	53.904	3.483	1.00	59.74		C
ATOM	2234	CD	ARG			57.137	54.136	2.871	1.00	58.42		C
ATOM	2235	NE	ARG			57.566	52.982	2.086	1.00	57.23		N
ATOM	2236	CZ	ARG			58.706	52.918	1.406	1.00			C
ATOM	2237		ARG			59.547	53.944	1.409	1.00			N
ATOM	2238		ARG			59.002	51.825	0.718	1.00	58.20		N
ATOM	2239	N			413	53.514	53.806	6.972	1.00	67.55		N
ATOM	2240	CA			413	53.480	52.643	7.851	1.00	70.19		C
ATOM	2241	C			413	52.367	52.630	8.894	1.00	72.70		C.
MOTA	2242	0			413	51.812	51.573	9.189	1.00			0
ATOM	2242	СВ			413	54.828	52.496	8.548	1.00	70.18		С
ATOM	2244	N			414	52.045	53.794	9.456	1.00	76.29		N
ATOM	2245	CA			414	51.020	53.864	10.492	1.00			C
ATOM	2245	C			414	49.605	53.528	10.021	1.00			C
MOTA	2247	0			414	48.799	53.012	10.803	1.00	80.83		0
ATOM	2248	СВ			414	51.033		11.184	1.00			С
MOTA	2249	CG			414	50.589	56.425	10.341		80.51		C
ATOM	2250	CD			414	50.376				81.22		C
ATOM	2251	NE			414	49.912	58.836	10.532		81.34		N
ATOM	2252	CZ			414	50.676	59.603	9.757		81.51		C
ATOM	2253		ARG			51.959	59.310	9.583		80.79		N
ATOM	2254		ARG			50.158	60.671	9.161		80.72		N
ATOM	2255		ASN			49.294	53.814	8.758		81.82		N
	2256	CA			415	47.965	53.499	8.240		83.15		C
ATOM	2250	CA			415	47.967	52.029	7.797		83.41		C
ATOM	2257	0			415	47.862	51.733	6.602		84.28		Ō
ATOM		CB			415	47.598	54.394	7.036		83.73		C
MOTA	2259					47.997	55.861	7.227		84.65		Ċ
ATOM	2260	CG			415	47.436		8.076		84.65		ō
ATOM	2261				415	48.969				85.41		N
ATOM	2262		ASN					8.758		82.63		N
ATOM	2263	N			416	48.101		8.465		82.02		C
ATOM	2264	CA			416	48.118				82.01		C
ATOM	2265	С	IKP	A	416	46.776	49.041	0.009	1.00	55.01		-

MOTA	2266	0	TRP	Α	416	46.228	49.228	9.896	1.00 82.27	0
ATOM	2267	CB	TRP	Α	416	49.268	48.998	9.236	1.00 79.66	C
MOTA	2268	CG	TRP	A	416	48.850	47.849	10.126	1.00 77.46	C
ATOM	2269	CD1				48.380	46.627	9.731	1.00 76.95	C
MOTA	2270	CD2	TRP			48.806	47.849	11.560	1.00 76.39	C
ATOM	2271	NE1	TRP			48.040	45.871	10.828	1.00 75.11	N `
	2272	CE2	TRP			48.290	46.595	11.963	1.00 75.43	C
MOTA			TRP			49.149	48.788	12.544	1.00 75.87	C
MOTA	2273	CE3						13.309	1.00 75.55	c
MOTA	2274	CZ2	TRP			48.107	46.256		1.00 75.33	C
ATOM	2275	CZ3	TRP			48.965	48.449	13.884	1.00 75.60	C
MOTA	2276	CH2	TRP			48.448	47.193	14.251		
MOTA	2277	N	PHE			48.725	67.124	8.023	1.00 82.88	N
MOTA	2278	CA	PHE			49.810	67.001	8.991	1.00 82.94	C
MOTA	2279	C	PHE	А	429	50.394	65.588	8.957	1.00 82.92	C
MOTA	2280	0	PHE	А	429	49.681	64.621	8.683	1.00 82.79	0
MOTA	2281	CB	PHE	Α	429	49.292	67.335	10.408	1.00 83.53	C
MOTA	2282	CG	PHE	A	429	48.135	66.455	10.870	1.00 83.27	С
MOTA	2283	CD1	PHE	Α	429	48.310	65.082	11.041	1.00 82.47	C
MOTA	2284	CD2	PHE	Α	429	46.883	67.010	11.141	1.00 82.83	C
ATOM	2285		PHE			47.263	64.261	11.473	1.00 81.70	C
ATOM	2286		PHE			45.819	66.202	11.580	1.00 82.89	С
ATOM	2287	CZ			429	46.014	64.819	11.745	1.00 82.38	С
ATOM	2288	N	GLU			51.693	65.468	9.221	1.00 82.60	N
ATOM	2289	CA			430	52.327	64.157	9.229	1.00 82.03	C
		C	GLU			53.060	63.870	10.528	1.00 81.40	C
ATOM	2290					53.285	64.769	11.340	1.00 81.74	Ō
ATOM	2291	0			430		64.703	8.069	1.00 80.59	C
MOTA	2292	CB			430	53.302		7.846	1.00 80.58	C
MOTA	2293	CG			430	53.725	62.546		1.00 79.33	C
ATOM	2294	CD			430	54.143	62.283	6.421		0
MOTA	2295					55.063	62.985	5.936	1.00 79.26	
MOTA	2296	OE2			430	53.547	61.382	5.773	1.00 78.51	0
MOTA	2297	N			431	53.456	62.614	10.712	1.00 79.43	N
MOTA	2298	CA	GLU	Α	431	54.133	62.214	11.941	1.00 77.44	C
MOTA	2299	C	GLU	Α	431	55.365	61.338	11.724	1.00 75.89	C
MOTA	2300	0	GLU	Α	431	· 55.739	60.568	12.606	1.00 75.77	0
MOTA	2301	CB	GLU	Α	43.1	53.129	61.482	12.841	1.00 76.96	. С
MOTA	2302	CG	GLU	Α	431	51.677	61.970	12.631	1.00 76.64	С
MOTA	2303	CD	GLU	Α	431	50.767	61.647	13.795	1.00 77.02	С
MOTA	.2304	OE1	GLU	Α	431	50.818	60.496	14.301	1.00 76.77	0.
MOTA	2305		GLU			49.984	62.546	14.214	1.00 77.41	0
ATOM	2306	N	GLY	A	432	56.000	61.462	10.562	1.00 74.32	N
ATOM	2307	CA			432	57.179	60.660	10.297	1.00 72.21	С
ATOM	2308	C			432	57.936	61.058	9.047	1.00 70.77	C
ATOM	2309	0			432	57.540	61.985	8.337	1.00 71.05	0
ATOM	2310	N			433	59.032	60.352	8.776	1.00 68.86	N
ATOM	2311	CA			433	59.855	60.629	7.603	1.00 66.42	C
	2312	C			433	60.245	59.353	6.852	1.00 64.76	С
MOTA		0			433	60.353	58.275	7.442	1.00 63.75	0
MOTA	2313						61.397	7.998	1.00 66.53	· C
ATOM	2314	CB			433	61.139		8.567	1.00 66.43	C
ATOM	2315		VAL			60.776	62.757		1.00 66.43	C
MOTA	2316		VAL			61.928	60.600	9.016		и
MOTA	2317	N			434	60.445	59.498	5.544	1.00 62.35	
MOTA	2318	CA			434	60.824	58.399	4.656	1.00 60.25	C
MOTA	2319	C			434	62.173	58.780	4.052	1.00 58.31	C
MOTA	2320	0			434	62.333	59.891	3.549	1.00 58.55	0
MOTA	2321	CB	ASP	A	434	59.780	58.260	3.539	1.00 61.48	C
ATOM	2322	CG	ASP	Α	434	59.952	56.994	2.715	1.00 62.63	С

ATOM	2323	OD1	ASP	A	434	61.091	56.500	2.578	1.00	65.25		0
ATOM	2324	OD2	ASP	Α	434	58.936	56.499	2.186	1.00	63.34		0
MOTA	2325	N	SER	Α	435	63.143	57.873	4.095	1.00	55.86		N
ATOM	2326	CA	SER	Α	435	64.459	58.182	3.548	1.00	53.85		C
ATOM	2327	С	SER	А	435	65.260	56.977	3.069		51.23		С
MOTA	2328	0	SER	A	435	64.753	55.859	2.996	1.00	50.16		0
ATOM	2329	CB	SER	Α	435	65.279	58.952	4.583	1.00	53.87		С
ATOM	2330	OG	SER	Α	435	65.363	58.220	5.792	1.00	56.33		0
MOTA	2331	N	TYR	A	436	66.523	57.230	2.744	1.00	49.98		N
MOTA	2332	CA	TYR	A	436	67.436	56.203	2.263	1.00	49.61		С
ATOM	2333	C	TYR	A	436	68.712	56.158.	3.104	1.00	48.71		С
MOTA	2334	0	\mathtt{TYR}	А	436	69.174	57.187	3.602	1.00	48.91		0
ATOM	2335	CB	TYR	Α	436	67.817	56.485	0.806	1.00	51.63		C
MOTA	2336	CG	TYR	A	436	66.691	56.313	-0.188	1.00	52.47		С
ATOM	2337	CD1	TYR	Α	436	66.256	55.044	-0.562	1.00	52.86		C
ATOM	2338	CD2	TYR	Α	436	66.058	57.420	-0.752	1.00	54.05		С
MOTA	2339	CE1	TYR	A	436	65.219	54.878	-1.475	1.00	55.19		С
ATOM	2340	CE2	TYR	Α	436	65.015	57.267	-1.668	1.00	55.67		С
MOTA	2341	CZ	TYR	Α	436.	64.602	55.992	-2.023	1.00	55.33	•	С
ATOM	2342	OH	TYR	А	436	63.569	55.825	-2.916	1.00	57.47		0
MOTA	2343	N	VAL	Α	437	69.272	54.963	3.263	1.00	45.78		N
MOTA	2344	CA	VAL	Α	437	70.514	54.794	4.008	1.00	44.47		С
MOTA	2345	C	VAL	Α	437	71.501	54.059	3.114	1.00	44.14		С
ATOM	2346	0	VAL			71.120	53.167	2.357	1.00	43.85		0
ATOM	2347	CB	VAL	Α	437	70.318	53.984	5.316	1.00	43.82		C
ATOM	2348	CG1	VAL			69.389	54.736	6.255		42.73		С
ATOM	2349	CG2	VAL	Α	437	69.778	52.598	5.004		41.37		С
ATOM	2350	N			438	72.788	54.429	3.186		44.43		N
ATOM	2351	CA	PRO			73.798	53.770	2.352		43.91		С
ATOM	2352	С			438	73.930	52.285	2.654		43.14		C
ATOM	2353	0	PRO			73.975	51.883	3.816		43.63		Ō
ATOM	2354	CB	PRO			75.073	54.556	2.667		44.21		C
ATOM	2355	CG	PRO			74.849	55.003	4.085		44.54		C
ATOM	2356	CD	PRO			73.403	55.436	4.070		43.37		Ċ
ATOM	2357	N	TYR			73.971	51.480	1.597		42.30		N
MOTA	2358	CA	TYR			74.103	50.034	1.713		41.24		C
MOTA	2359	С	TYR			75.441	49.711	2.362		42.01		C
MOTA	2360	0	TYR		•	76.477	50.233	1.956		41.44		ō
ATOM	2361	CB	TYR			74.025	49.391	0.323		39.97	, ,	C
ATOM	2362	CG	TYR			74.174	47.884	0.302		37.05		C
ATOM	2363		TYR			73.341	47.067	1.063		37.13		C
MOTA	2364		TYR			75.134	47.273	-0.506		38.06		C
MOTA	2365		TYR			73.458	45.675	1.019		37.56		C
ATOM	2366	CE2				75.260	45.887	-0.557		36.89		C
MOTA	2367	CZ	TYR			74.419	45.094	0.206		38.34		C
ATOM	2368	OH	TYR			74.544	43.723	0.158		39.52		0
ATOM	2369	N	ALA			75.415	48.841	3.366		42.74		N
ATOM	2370	CA	ALA			76.632	48.473	4.078		42.66		C
MOTA	2371	C	ALA			76.991	47.007	3.907		42.37		C
MOTA	2372	0	ALA			77.982	46.540	4.462		43.02		ō
ATOM	2373	CB	ALA			76.480	48.799	5.561		42.72		C
ATOM	2374	N	GLY			76.190	46.282	3.139		41.94		N.
ATOM	2375	CA	GLY			76.465	44.872	2.940		41.40		C
ATOM	2376	C	GLY			75.788	44.014	3.991		42.16		C
ATOM	2377	0	GLY			74.776	44.410	4.568		42.14		o
ATOM	2378	N	LYS			76.351	42.838	4.246		42.68		N
ATOM	2379	CA	LYS			75.799	41.909	5.225		42.67		C
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ATOM	2380	С	LYS	A	442	76.048	42.345	6.675	1.00	41.33		C
MOTA	2381	0	LYS	A	442	77.086	42.924	7.000	1.00	39.63		0
MOTA	2382	CB	LYS	А	442	76.384	40.515	4.990	1.00	45.23		С
MOTA	2383	CG	LYS	Α	442	76.063	39.949	3.612	1.00	49.35		C
ATOM	2384	CD	LYS	Α	442	74.990	38.864	3.670		51.07		С
MOTA	2385	CE	LYS	A	442	75.563	37.563	4.226	1.00	54.09		C
MOTA	2386	NZ	LYS	Α	442	74.589	36.429	4.216	1.00	55.56		N
MOTA	2387	N	LEU			75.078	42.055	7.534	1.00	40.11		N
MOTA	2388	CA	LEU	A	443	75.140	42.395	8.951	1.00	38.38		C
MOTA	2389	С	LEU			76.422	41.932	9.657	1.00	38.75		C
MOTA	2390	0	LEU			77.085	42.717	10.329	1.00	36.60		0
MOTA	2391	CB	LEU			73.917	41.805	9.659	1.00	35.66		C
ATOM	2392	CG	LEU			73.769	41.987	11.173		34.22		C
MOTA	2393		LEU			72.311	41.806	11.567	1.00	31.06		C
ATOM	2394	CD2	LEU			74.660	40.991	11.904	1.00	33.38		С
ATOM	2395	N	LYS	A	444	76.763	40.659	9.489	1.00	39.50		N
MOTA	2396	CA	LYS			77.939	40.065	10.125	1.00	42.18		С
MOTA	2397	C	LYS	А	444	79.232	40.890	10.156	1.00	41.66		С
MOTA	2398	0	LYS	A	444	79.745	41.200	11.229	1.00	42.08		0
MOTA	23.99	CB	LYS	A.	444	78.237	38.702	9.493	1.00	43.45		С
MOTA	2400	CG	LYS	Α	444	79.237	37.878	10.285	1.00	48.67		C
MOTA	2401	CD	LYS	Α	444	79.460	36.511	9.663	1.00	51.53	•	C
MOTA	2402	CE	LYS	Α	444	80.285	35.630	10.585	1.00	52.97		C
MOTA	2403	NZ	LYS	A	444	81.600	36.254	10.907	1.00	53.80		N
MOTA	2404	N	ASP	А	445	79.757	41.240	8.988	1.00	41.15		N
MOTA	2405	CA	ASP	Α	445	81.005	41.991	8.901	1.00	41.12		C
MOTA	2406	C	ASP	Α	445	80.951	43.355	9.567	1.00	40.48		C
MOTA	2407	0	ASP	Α	445	81.936	43.810	10.149	1.00	39.71		0
ATOM	2408	CB	ASP	Α	445	81.412	42.164	7.436	1.00	44.73		C
ATOM	2409	CG	ASP	Α	445	81.511	40.841	6.698	1.00	47.59		С
MOTA	2410	OD1	ASP	Α	445	82.364	40.008	7.077	1.00	48.96		0
ATOM	2411	OD2	ASP	A	445	80.726	40.636	5.746	1.00	50.74		0
ATOM	2412	N	ASN	A	446	79.802	44.012	9.471 ՝	1.00	38.11		N
ATOM	2413	CA	ASN	Α	446	79.637	45.332	10.058	1.00	37.61		C
MOTA	2414	С	ASN	Α	446	79.543	45.289	11.579	1.00	37.06		C
MOTA	2415	0	ASN	Α	446	80.122	46.136	12.261	1.00	35.82		0
ATOM	2416	CB	ASN	A	446	78.405	46.000	9.469	1.00	38.33		C
MOTA	2417	CG	ASN	Α	446	78.605	46.388	8.023	1.00	39.42		С
ATOM	2418	OD1	ASN	Α	446	79.106	47.473	7.725	1.00	39.50		0
MOTA	2419	ND2	ASN	Α	446	78.232	45.493	7.112	1.00	38.24		N
MOTA	2420	N	VAL	Α	447	78.815	44.309	12.106	1.00	35.62		N
MOTA	2421	CA	VAL	Α	447	78.676	44.165	13.547	1.00	36.21		C
MOTA	2422	С	VAL	Α	447	80.030	43.786	14.160	1.00	36.80		C
MOTA	2423	0	VAL	A	447	80.419	44.314	15.199	1.00	36.29		0
MOTA	2424	CB	VAL	Α	447	77.629	43.087	13.901	1.00	35.55		C
MOTA	2425	CG1	VAL	A	447	77.741	42.707	15.373	1.00	34.78		С
MOTA	2426	CG2	VAL	А	447	76.229	43.612	13.598	1.00	34.46		C
MOTA	2427	N	GLU	А	448	80.746	42.876	13.505	1.00	37.04	•	N
ATOM .	2428	CA	GLU	Α	448	82.048	42.451	13.994	1.00	38.35		С
MOTA	2429	C	GLU	Α	448	82.967	43.667	14.076	1.00	36.95		С
MOTA	2430	0	GLU	Α	448	83.655	43.864	15.075	1.00	35.90		0
MOTA	2431	CB	GLU	A	448	82.656	41.392	13.062	1.00	40.48		C
MOTA	2432	CG	GLU	Α	448	83.949	40.772	13.586	1.00	45.60		C
MOTA	2433	CD	GLU	Α	448	84.553	39.739	12.634	1.00	50.26		C
MOTA	2434		GLU			85.094	40.133	11.573	1.00	51.53		0
ATOM	2435	OE2	GLU	A	448	84.482	38.529	12.950	1.00	52.94		0
MOTA	2436	N	ALA	Α	449	82.960	44.485	13.028	1.00	34.49		N

MOTA	2437	CA	ALA	Α	449	83.793	45.683	12.982	1.00 34.45		C
ATOM	2438	C	ALA	Α	449	83.417	46.670	14.089	1.00 33.89		C
MOTA	2439	0	ALA	Α	449	84.282	47.195	14.790	1.00 33.96		0
MOTA	2440	CB	ALA	Α	449	83.665	46.361	11.616	1.00 34.26		С
MOTA	2441	N	SER	Α	450	82.123	46.924	14.233	1.00 31.81		N
ATOM	2442	CA	SER	А	450	81.638	47.841	15.252	1.00 32.08		. C
MOTA	2443	С	SER			82.023	47.380	16.657	1.00 31.86		C
ATOM	2444	0	SER			82.531	48.166	17.463	1.00 29.55		0
ATOM	2445	CB	SER			80.112	47.969	15.167	1.00 30.70		C
ATOM	2446	OG	SER			79.724	48.753	14.056	1.00 31.66		0
ATOM	2447	N	LEU			81.784	46.103	16.941	1.00 31.11		N
ATOM	2448	CA:	LEU			82.077	45.556	18.259	1.00 32.52		C
ATOM	2449	C	LEU			83.565	45.413	18.559	1.00 33.63		C
ATOM	2450	0	LEU			83.959	45.383	19.723	1.00 33.14		0
	2451	CB	LEU			81.347	44.227	18.449	1.00 30.21		Ċ
ATOM			LEU			79.824	44.407	18.426	1.00 30.73		Ċ
ATOM	2452	CG				79.143	43.096	18.766	1.00 27.89		C
ATOM	2453		LEU			79.143	45.501	19.416	1.00 27.03		C
ATOM	2454		LEU						1.00 25.00		N
ATOM	2455	N	ASN			84.392	45.331	17.521			C
ATOM	2456	CA	ASN			85.831	45.251	17.732	1.00 35.86 1.00 35.32		C
ATOM	2457	C ·			452	86.294	46.601	18.274			
MOTA	2458	0	ASN			87.176	46.665	19.134	1.00 34.79		0
MOTA	2459	CB	ASN			86.581	44.941	16.429	1.00 37.41		C
MOTA	2460	CG	ASN			86.632	43.459	16.125	1.00 41.69		C
MOTA	2461		ASN			86.668	42.626	17.037	1.00 45.32		0
MOTA	2462	ND2	ASN			86,656	43.117	14.841	1.00 44.05		N
MOTA	2463	N	LYS	Α	453	85 [.] .695	47.680	17.774	1.00 34.56	•	N
MOTA	2464	CA	LYS	Α	453	86.069	49.012	18.235	1.00 35.20		C
MOTA	2465	C	LYS	Α	453	85.568	49.255	19.651	1.00 32.43		C
MOTA	2466	0	LYS	A	453	86.237	49.915	20.442	1.00 31.92		0
MOTA	2467	CB	LYS	Α	453	85.533	50.098	17.292	1.00 36.51		С
ATOM	2468	CG	LYS	Α	453	86.090	49.988	15.877	1.00 42.24		C
ATOM	2469	CD	LYS	Α	453	86.165	51.338	15.160	1.00 43.06		C
ATOM	2470	CE	LYS	Α	453	84.835	52.050	15.172	1.00 45.98		C
ATOM	2471	NZ	LYS	Α	453	84.889	53.331	14.419	1.00 46.25		N
ATOM	2472	N	VAL	Α	454	84.391	48.724	19.968	1.00 30.18		N
ATOM	2473	CA	VAL	Α	454	83.836	48.878	21.303	1.00 28.56		C
ATOM	2474	С	VAL	Α	454	84.741	48.143	22.295	1.00 29.40		C
ATOM	2475	0	VAL	A	454	85.100	48.690	23.338	1.00 26.82		0
ATOM	2476	CB	VAL	A	454	82.401	48.306	21.390	1.00 29.78		С
ATOM	2477		VAĻ			81.943	48.247	22.855.	1.00 26.04		C
ATOM	2478				454	81.444	49.181	20.572	1.00 29.03	•	С
MOTA	2479	N			455		46.910	21.953	1.00 28.71		N
ATOM	2480	CA			455		46.095	22.799	1.00 30.25		C
ATOM	2481	C			455		46.774	23.020	1.00 30.25		С
ATOM	2482	0.			455	87.864	46.779	24.125	1.00 29.71		0
ATOM	2483	CB			455		44.725	22.159	1.00 29.78		С
ATOM	2484	CG			455		43.776	22.199	1.00 31.31		C
ATOM	2485	CD			455		42.555	21.340	1.00 34.36		C
ATOM	2486	CE			455	84.234	41.536	21.385	1.00 38.66		Ċ
						84.480	40.397	20.448	1.00 40.02		N
ATOM	2487	NZ N			455 456	87.876	47.338	21.950	1.00 40.02		N
ATOM	2488	N CA			456			22.012	1.00 31.20		C
ATOM	2489	CA			456	89.159	48.020	22.012	1.00 32.86		C
ATOM	2490	C			456	89.063	49.232		1.00 32.37		0
ATOM	2491	0			456	89.938	49.461	23.786			C
ATOM	2492	CB			456	89.583	48.453	20.601	1.00 33.72		0
MOTA	2493	OG	SER	A	456	90.866	49.044	20.615	1.00 36.70		O

MOTA	2494	N	THR	А	457	87.994	50.009	22.776	1.00 29.64	N
ATOM	2495	CA	THR	Α	457	87.787	51.178	23.614	1.00 29.25	Ċ
MOTA	2496	C	THR	A	457	87.595	50.733	25.060	1.00 28.90	C.
MOTA	2497	0	THR	Α	457	88.086	51.380	25.981	1.00 28.75	0
MOTA	2498	CB	THR			86.561	51.982	23.158	1.00 29.05	С
MOTA	2499	OG1	THR			86.757	52.393	21.805	1.00 32.49	0
MOTA	2500	CG2	THR			86.369	53.216	24.022	1.00 26.06	С
MOTA	2501	N	MET			86.884	49.625	25.259	1.00 28.56	N
MOTA	2502	CA	MET			86.663	49.111	26.603	1.00 27.60	С
ATOM	2503	С	MET			87.993	48.832	27.288	1.00 28.20	C
ATOM	2504	0	MET			88.167	49.155	28.459	1.00 28.30	0
ATOM	2505	CB	MET			85.792	47.853	26.560	1.00 27.08	C
ATOM	2506	CG	MET			84.306	48.170	26.380	1.00 26.92	C
ATOM	2507	SD	MET			83.227	46.746	26.210	1.00 28.93	S
ATOM	2508	CE	MET			83.415	45.945	27.805	1.00 27.06	C
ATOM	2509	N			459	88.944	48.252	26.561	1.00 29.24	N
MOTA	2510	CA			459	90.254	47.982	27.141	1.00 30.30	C
MOTA	2511	C			459	91.009	49.273	27.466	1.00 30.36	C
MOTA	2512	0			459	91.818	49.303	28.397	1.00 28.82	0
ATOM	2513	CB			459	91.092	47.100	26.212	1.00 32.96	C S
MOTA	2514	SG	ASN		459	90.670	45.337	26.352	1.00 36.19 1.00 28.82	N
MOTA	2515	N CA				90.757 91.411	50.335	26.702 26.986	1.00 28.82	C
ATOM ATOM	2516 2517	CA	ASN ASN			90.884	51.609 52.087	28.334	1.00 29.47	C
ATOM	2518	0	ASN				52.756	29.079	1.00 28.39	0
ATOM	2519	CB	ASN			91.586 91.078	52.730	25.937	1.00 29.43	C
ATOM	2520	CG	ASN			91.076	52.434	24.610	1.00 23.45	, C
MOTA	2521		ASN			91.730	52.161	23.612	1.00 32.43	0
ATOM	2522		ASN			93.080	52.536	24.589	1.00 33.79	N
ATOM	2523	N			461	89.636	51.735	28.633	1.00 31.09	N
ATOM	2524	CA	CYS			88.993	52.143	29.878	1.00 27.53	C
ATOM	2525	C			461	89.204	51.138	31.010	1.00 27.92	C
ATOM	2526	0			461	88.633	51.289	32.086	1.00 27.95	ō
ATOM	2527	СВ			461	87.486	52.355	29.646	1.00 29.51	C
ATOM	2528	SG			461	87.070	53,620	28.389	1.00 32.81	s
ATOM ·	2529	N			462	90.021	50.119	30.762	1.00 27.78	N
ATOM	253.0	CA			462	90.293	49.106	31.767	1.00 27.70	С
ATOM	2531	С			462	89.133	48.163	32.052	1.00 28.72	С
MOTA	2532	0			462	88.987	47.674	33.176	1.00 29.35	0
MOTA	2533	N	ALA			88.315	47.881	31.043	1.00 27.30	N
ATOM	2534	CA.	ALA	Α	463	87.163	47.012	31.248	1.00 27.53	С
MOTA	2535	C	ALA	Α	463	87.121	45.785	30.352	1.00 27.82	С
MOTA	2536	0	ALA	A	463	87.288	45.886	29.139	1.00 27.55	0
MOTA	2537	CB	ALA	Α	463	85.879	47.820	31.069	1.00 26.38	С
MOTA	2538	N			464	86.884	44.628	30.961	1.00 28.56	N
ATOM	2539	CA			464	86.785	43.369	30.223	1.00 30.06	C
MOTA	2540	C	LEU	Α	464	85.330	42.963	30.014	1.00 29.07	C
MOTA	2541	0	LEU	Α	464	85.043	42.046	29.246	1.00 31.05	0
ATOM	2542	CB	LEU	А	464	87.512	42.237	30.961	1.00 31.49	C
ATOM	2543	CG	LEU	Α	464	88.993	42.025	30.640	1.00 33.97	. С
MOTA	2544		LEU			89.150	41.723	29.158	1.00 36.04	С
MOTA	2545	CD2	LEU			89.788	43.265	31.004	1.00 38.27	С
ATOM	2546	N			465	84.419	43.633	30.712	1.00 27.77	N
ATOM	2547	CA			465	82.996	43.338	30.595	1.00 27.41	С
ATOM	2548	C			465	82.197	44.630	30.674	1.00 27.20	C
ATOM	2549	0			465	82.709	45.664	31.107	1.00 26.83	0
MOTA	2550	CB	THR	A	465	82.494	42.417	31.736	1.00 27.84	С

ATOM	2551	OG1	THR	Α	465	82.536	43.133	32.975	1.00 28.30		0
ATOM	2552		THR			83.355	41.159	31.838	1.00 28.72		С
ATOM	2553	N.	ILE			80.936	44.567	30.260	1.00 25.31		N
ATOM	2554	CA	ILE			80.085	45.743	30.298	1.00 25.03		С
ATOM	2555	C	ILE			79.898	46.236	31.732	1.00 24.87		С
MOTA	2556	0	ILE			79.985	47.430	31.993	1.00 27.04		0
	2557	CB	ILE			78.724	45.456	29.629	1.00 25.22		С
ATOM		CG1				78.939	45.313	28.114	1.00 24.45		C
ATOM	2558					77.726	46.565	29.944	1.00 22.53		C
ATOM	2559	CG2	ILE			77.699	44.908	27.350	1.00 25.70		C
ATOM	2560		PRO			79.638	45.327	32.684	1.00 25.70		N
ATOM	2561	N				79.468	45.805	34.058	1.00 25.31		C
ATOM	2562	CA	PRO				46.506	34.570	1.00 26.95		C
ATOM	2563	C	PRO			80.730	47.499	35.292	1.00 20.35		ō
ATOM	2564	0	PRO			80.649			1.00 27.33	•	C
ATOM	2565	CB	PRO			79.149	44.525	34.828	1.00 24.45		C
ATOM	2566	CG	PRO			78.393	43.723	33.811	1.00 24.43		C
MOTA	2567	CD	PRO			79.258	43.909	32.577			И
MOTA	2568	N	GLN			81.897	46.003	34.186	1.00 27.99		C
MOTA	2569	CA	GLN			83.137	46.623	34.630	1.00 28.59		
MOTA	2570	С	GLN			83.320	47.995	33.976	1.00 29.85		C
MOTA	2571	0	GLN			83.844	48.926	34.594	1.00 29.02		0
MOTA	2572	CB	GLN			84.320	45.710	34.323	1.00 29.66		C
MOTA	2573	CG	GLN			85.623	46.216	34.879	1.00 30.83		C
MOTA	2574	CD			468	86.722	45.175	34.834	1.00 29.49		С
MOTA	2575	OE1	GLN	A	468	86.806	44.380	33.900	1.00 27.39		0
MOTA	2576	NE2	GLN	Α	468	87.589	45.194	35.839	1.00 32.22		N
MOTA	2577	N	LEU	Α	469	82.872	48.124	32.729	1.00 28.18		N
MOTA	2578	CA	LEU	Α	469	82.961	49.395	32.025	1.00 26.94		C
ATOM	2579	С	LEU	Α	469	82.029	50.413	32.676	1.00 27.29		C
MOTA	2580	0	LEU	A	469	82.379	51.587	32.815	1.00 26.46		0
MOTA	2581	CB	LEU	A	469	82.566	49.232	30.554	1.00 27.22		C
ATOM	2582	CG	LEU	Α	469	82.343	50.536	29.777	1.00 28.28		С
ATOM	2583	CD1	LEU	Α	469	83.683	51.232	29.552	1.00 25.24		С
MOTA	2584	CD2	LEU	A	469	81.657	50.238	28.438	1.00 27.64		С
ATOM.	2585	N	GLN	A	470	80.845	49.959	33.076	1.00 26.40		N
ATOM	2586	CA	GLN	A	470	79.864	50.851	33.685	1.00 28.89		C
MOTA	2587	C	GLN	Α	470	80.344	51.351	35.038	1.00 29.84		С
ATOM	2588	0	GLN	Α	470	80.001	52.444	35.480	1.00 28.12		0
ATOM	2589	CB	GLN	A	470	78.513	50.132	33.807	1.00 27.17		С
ATOM	2590	CG			470	77.962	49.716	32.434	1.00 27.68		C
ATOM	2591	CD	GLN	А	470	76.666	48.938	32.506	1.00 28.13		С
ATOM	2592		GLN			76.449	48.166	33.432	1.00 28.58		0
MOTA	2593	NE2			470	75.803	49.122	31.508	1.00 26.29		N
ATOM	2594	N			471	81.173	50.543	35.676	1.00 31.64		N
ATOM	2595	CA			471	81.712	50.880	36.976	1.00 31.86		C
ATOM	2596	C			471	82.949	51.783	36.887	1.00 32.13		C
MOTA	2597	Ō			471	83.081	52.742	37.646	1.00 32.18		0
MOTA	2598	СВ			471	82.050	49.585	37.722	1.00 30.51		С
ATOM	2599	OG			471	82.831	49.842	38.870	1.00 33.39		0
ATOM	2600	N			472	83.830	51.493	35.936	1.00 32.80		N
ATOM	2601	CA			472	85.081	52.234	35.783	1.00 33.19		С
ATOM	2601	C			472	85.148	53.388	34.781	1.00 32.28		C
ATOM	2602	0			472	86.097	54.163	34.813	1.00 32.33		Ō
	2603	CB			472	86.201	51.245	35.452	1.00 34.04		C
ATOM	2604	CG			472	86.335	50.127	36.466	1.00 36.23		C
MOTA	2605	CD			472	87.335	49.075	36.019	1.00 38.07		C
ATOM		CE			472	88.755	49.592	36.059	1.00 39.38		C
MOTA	2607	CE	пго	A	4/4	00.755	-	30.039	2.00 32.30		-

MOTA	2608	NZ	LYS	Α	472	89.723	48.517	35.698	1.00 41.01	N
MOTA	2609	N	ALA	Α	473	84.170	53.506	33.889	1.00 31.34	N
ATOM	2610	CA	ALA	Α	473	84.201	54.572	32.892	1.00 30.17	С
ATOM	2611	С	ALA	Α	473	84.324	55.987	33.461	1.00 30.11	С
ATOM	2612	0	ALA	А	473	83.718	56.334	34.480	1.00 30.70	0
MOTA	2613	CB			473	82.971	54.489	31.986	1.00 29.13	C
ATOM	2614	N			474	85.136	56.788	32.781	1.00 30.05	N
ATOM	2615	CA			474	85.362	58.184	33.129	1.00 29.85	C
ATOM	2616	C			474	84.772	58.909	31.928	1.00 29.93	C
ATOM	2617	Õ			474	85.302	58.833	30.816	1.00 29.14	0
ATOM	2618	CB			474	86.862	58.441	33.277	1.00 29.14	C
ATOM	2619	CG			474			34.471		
ATOM	2620	CD			474	87.460	57.684	34.471	1.00 28.70 1.00 27.54	C
ATOM						88.943	57.375			. C
	2621	CE			474	89.803	58.620	34.334	1.00 29.17	C
ATOM	2622	NZ			474	91.222	58.265	34.018	1.00 28.64	N
ATOM	2623	N			475	83.660	59.597	32.150	1.00 29.12	N
ATOM	2624	CA			475	82.968	60.254	31.056	1.00 29.85	C
ATOM	2625	C			475	82.935	61.764	31.176	1.00 29.94	С
ATOM	2626	0			475		62.314	32.166	1.00 30.35	0
ATOM	2627	CB			475	81.524	59.703	30.943	1.00 29.86	. C
MOTA	2628	CG1	ILE			81.564	58.164	30.940	1.00 29.42	C
MOTA	2629	CG2	ILE	Α	475	80.867	60.213	29.666	1.00 29.91	C
MOTA	2630	CD1	ILE	Α	475	80.205	57.470	30.951	1.00 23.94	C
ATOM	2631	N	THR	Α	476	83.459	62.429	30.1/53	1.00 29.56	N
MOTA	2632	CA	THR	Α	476	83.511	63.881	30.141	1.00 29.14	C
MOTA	2633	С	THR	Α	476	82.686	64.506	29.042	1.00 28.15	C
ATOM	2634	0	THR	Α	476	82.582	63.986	27.932	1.00 26.60	0
ATOM	2635	CB	THR	A	476	84.962	64.414	29.981	1.00 28.25	С
ATOM	2636	OG1	THR	Α	476	84.953	65.844	30.066	1.00 32.24	0
ATOM	2637	CG2	THR			85.535	64.022	28.629	1.00 26.65	C
ATOM	2638	N	LEU			82.105	65.644	29.381	1.00 29.09	N
ATOM ·	2639	CA	LEU			81.312	66.424	28.456	1.00 32.22	C
ATOM	2640	C	LEU			82.352	67.281	27.731	1.00 32.43	C
ATOM	2641	Ō	LEU			83.395	67.592	28.304	1.00 32.10	0
ATOM	2642	СВ	LEU			80.352	67.312	29.256	1.00 33.05	C
MOTA	2643	CG	LEU			79.239	68.097	28.566	1.00 35.03	C
MOTA	2644		LEU			78.264	67.138	27.910	1.00 33.08	C
ATOM	2645		LEU			78.526	68.966	29.604	1.00 32.36	C
ATOM		N	VAL			82.093	67.635		1.00 33.80	
ATOM	2647	CA	VAL					26.477 25.726		N
ATOM	2648					83.018	68.480		1.00 35.55	C
		C	VAL			82.280	69.767	25.365	1.00 35.88	C
MOTA	2649	0	VAL			81.052	69.787	25.304	1.00 35.41	0
MOTA	2650	CB	VAL			83.516	67.796	24.422	1.00 36.48	C
ATOM	2651		VAL			83.960	66.370	24.718	1.00 37.57	C
ATOM	2652		VAL			82.428	67.822	23.363	1.00 38.80	C
ATOM	2653	N	SER			83.028	70.839	25.132	1.00 37.26	N
ATOM	2654	CA	SER			82.432	72.127	24.794	1.00 39.38	C
ATOM	2655	C	SER			81.806	72.119	23.406	1.00 40.82	C
MOTA	2656	0	SER	Α	479	82.200	71.341	22.537	1.00 41.28	0
MOTA	2657	CB	SER	A	479	83.488	73.230	24.869	1.00 38.01	C
ATOM	2658	OG	SER	A	479	84.515	72.999	23.924	1.00 38.36	0
MOTA	2659	N	SER	Α	480	80.825	72.990	23.203	1.00 44.34	N
MOTA	2660	CA	SER	A	480	80.152	73.083	21.912	1.00 48.75	С
MOTA	2661	C	SER	А	480	81.149	73.491	20.828	1.00 50.10	C
MOTA	2662	0	SER			81.088	73.005	19.698	1.00 50.70	0
MOTA	2663	CB	SER			79.017	74.104	21.986	1.00 49.74	C
ATOM	2664	OG	SER			79.516	75.382	22.326	1.00 52.76	Õ
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MOTA	2665	N	VAL	А	481	8	32.074	74	.377	21	.187	1.	00	52.36		•	Ν.
MOTA	2666	CA	VAL	А	481	8	33.096	74	.856	20	.262	1.	00	54.26			C
ATOM	2667	C	VAL	Α	481	8	33.975	73	.729	19	.720	1.	00	55.31			C
MOTA	2668	0	VAL	А	481		34.319	73	.721	18	.537	1.	00	55.24			0
MOTA	2669	CB	VAL	Α	481	8	34.017	75	.901	20	.937	1.	00	54.94			C
MOTA	2670	CG1	VAL	Α	481	8	35.189	76	.234	. 20	.021	1.	00	55.96			C
ATOM	2671	CG2	VAL	Α	481	8	33.229	77	.162	21	.256	1.	00	55.59			С
ATOM	2672	N	SER				34.343	72	.788	20	.586	1.	00	56.16			N
ATOM	2673	CA	SER				35.190	71	.670		.183	1.	00	58.27			C
ATOM	2674	С	SER				34.491		.750		.184	1.	00	60.34			C
ATOM	2675	0	SER				35.144		.962		.493	1.	00	60.26			0
	2676	CB	SER				35.620	70	.855		.408			57.59			C
ATOM	2677	OG	SER				84.518		.189		.998			57.44			0
MOTA	2678	N	ILE				33.166		.851		.107			61.66			N
ATOM	2679	CA	ILE				32.395		.016		.192			64.37			C
ATOM	2680	C	ILE				32.307		637		.795			65.60			C
ATOM	2681	0	ILE				32.290		. 886		.692			65.96			ō
ATOM	2682	СВ	ILE				30.959		786		.728			64.32			C
ATOM	2683	CG1					31.023		252		.161			64.61			C
		CG2					30.215		3.796		.835			64.26			. C
MOTA	2684		ILE				79.670				.789			64.99			C
ATOM	2685	CDI	ILE				19.670	00	3.993	20	. 103	Ι.	00	04.55			C
TER	2686	**	ILE				-0 040	٠,			242	^	76	25 52			K
HETATM		K		А	900		52.942		264		.342			35.52			P
HETATM		P	IMP		602		57.729		5.171		.018			32.01			
HETATM		01P			602		57.318		5.116		.589			35.06			0
HETATM			IMP		602		58.541		.958		.324			37.34			0
HETATM			IMP		602		58.509		.460		.351			34.23			0
HETATM		05*	IMP	,	602		66.513		5.208		.042			32.49	•		0
HETATM		C5*	IMP		602		65.484		1.230		.900			28.06			C
HETATM		C4 *	IMP		602		54.416		1.369		.948			29.30			C
HETATM	2695	04*	IMP		602		63.654		5.545		.512			28.92			0
HETATM	2696	C3 *	IMP		602		63.350	53	3.301	17	.112			2 7. 97			С
HETATM	2697	03*	IMP		602		63.765	52	2.190	17	.882			29.87			0
HETATM	2698	C2*	IMP		602		62.219	54	1.048	17	7.747	1.	00	28.37			C
HETATM	2699	Q2*	IMP		602		62.308	54	1.094	19	.151	1.	00	28.77			0
HETATM	2700	C1*	IMP		602		62.341	55	5.422	17	.066	1.	00	29.44			C
HETATM	2701	N9	IMP		602		61.392	55	5.563	15	.918	1.	00	31.97			N
HETATM	2702	C8	IMP		602		60.890	54	1.644	15	.016	1.	00	32.78			C
HETATM	2703	N7	IMP		602		60.086	5	5.173	-14	.154	ĺ.	00	32.55			N
HETATM	2704	C5	IMP		602	•	60.027	56	5.497	.14	.463	1	00	34.42			C
HETATM		C6	IMP		602		59.302	5	7.582	13	.855	1.	00	35.14			C
HETATM	2706	06	IMP		602		58.555	5	7.521	12	2.883	1.	00	36.42			0
HETATM	2707	N1	IMP		602	•	59.516	58	3.848	_ 14	.495	1.	00	36.83			N
HETATM	2708	C2	IMP		602		60.355		9.011	15	.609	1.	00	38.21			C
HETATM	2709	N3	·IMP		602		61.034	5	7.973		5.170			35.63			N
HETATM		C4	IMP		602		60.832		5.774		5.563	1.	00	34.37			С
HETATM		0	нон		1		63.019		3.881		3.340			44.26			0
HETATM			нон		2		52.277		7.766		3.053			120.54			0
HETATM		0	нон		3		66.605		7.974		3.976			25.54			0
HETATM		Ö	НОН		4		59.386		5.205		5.943			29.43			0
HETATM		0	нон		5		79.662		1.845		.507			22.13			Ō
HETATM		0	нон		6		65.938		0.529		1.679			31.17			Ö
HETATM		0	нон		7		74.980		5.671		2.871			30.42			Ö
HETATM		0	НОН		8		57.548		3.753		3.347			28.92			Ô
		0			9		70.703		4.421		1.919			26.74			0
HETATM			HOH											27.12			0
HETATM		0	HOH		10		70.985 45.680		3.252		2.290						0
HETATM	2/21	0	нон		11		45.680	4	4.301	ТЛ	1.265	Ι.	UU.	103.96			U

HETATM	2722	0	нон	12	77.744	53.946	34.272	1.00	32.08		0
HETATM	2723	0	HOH	13	58.727	51.272	23.006	1.00	27.53		0
HETATM	2724	0	HOH	14	62.326	38.666	34.100	1.00	27.41		0
HETATM	2725	0	HOH	15	56.691	78.735	34.475	1.00	29.79		0
HETATM	2726	0	HOH	16	88.368	53.773	33.242	1.00	29.09		0
HETATM	2727	0	HOH	17	72.567	38.252	33.805	1.00	32.29		0
HETATM	2728	0	нон	18	87.198	55.495	31.179	1.00	28.25		0
HETATM	2729	0	HOH	19	49.308	44.270	21.126	1.00	33.03		0
HETATM	2730	0	нон	20 -	78.730	48.078	37.343	1.00	33.84		0
HETATM	2731	0	HOH	21	73.616	57.426	36.203	1.00	27.28		0
HETATM	2732	0	HOH	22	56.311	77.113	37.092	1.00	34.13		0
HETATM	2733	0	HOH	23	74.197	59.875	37.788	1.00	40.63		0
HETATM	2734	0	HOH	24	64.449	41.371	7.872	1.00	35.33		0
HETATM	2735	0	нон	25	76.108	43.846	30.984	1.00	26.68		0
HETATM	2736	0	нон	26	70.175	33.467	27.535	1.00	36.79		0
HETATM	2737	0	нон	27	84.289	53.139	21.052	1.00	32.01		0
HETATM	2738	0	нон	28	56.502	57.506	38.867	1.00	42.20		0
HETATM	2739	0	НОН	29	48.256	54.233	36.924	1.00	41.83		0
HETATM	2740	0	нон	30	75.042	38.867	31.153	1.00	33.27		0
HETATM	2741	0	НОН	31	69.348	62.804	21.515		38.19		0
HETATM	2742	0	НОН	32	92.355	40.593	20.080		59.23		0
HETATM		O	нон	33	59.908	50.926	20.187		37.89		0
HETATM		0	НОН	34	53.040	51.707	38.077		33.13		0
HETATM	2745	0	HOH	35	58.612	45.227	6.010	1.00	41.56		Ō
HETATM		0	НОН	36	69.127	67.876	32.847		41.45		Ō
HETATM		0	НОН	37	63.999	56.486	20.273		37.87		Ō
HETATM		0	НОН	38	52.165	53.830	25.868		36.90		ō
HETATM		0	нон	39	65.226	36.648	34.797		33.52		Ō
HETATM		0	нон	40	67.969	38.369	46.331		38.33		ō
HETATM		0	нон	41	76.432	41.259	32.168		31.45		Ō
HETATM		0	нон	42	58.931	42.035	5.988		51.68		ō
HETATM		0	НОН	43	58.873	38.279	34.683		31.39		ō
HETATM		0	НОН	44	91.268	41.892	34.973		45.58		Ō
HETATM		0	нон	45	87.214	67.124	30.708		29.61		Ō
HETATM		0	нон	46	61.767	50.507	18.007		29.58		0
HETATM	2757	0	нон	47	53.679	55.874	20.408	1.00	48.69		0
HETATM	2758	0	НОН	48	56.278	41.477	37.489	1.00	44.57		0
HETATM	2759	0	НОН	49	59.791	59.574	31.027	1.00	52.11		0
HETATM	2760	0	НОН	50	62.820	39.505	6.099		44.52		0
HETATM	2761	0	нон	51		43.256	7.770	1.00	52.85		0
HETATM		0	нон	52	58.407	35.678	26.960		39.42		0
HETATM	2763	0	нон	53	59.608	51.214	9.860	1.00	33.11		0
HETATM	2764	0	нон	54	59.577	51.575	16.371		31.46		0
HETATM	2765	0	НОН	55	74.077	50.717	36.341	1.00	43.49		0
HETATM	2766	0	нон	56	79.182	38.296	17.383	1.00	40.40		0
HETATM	2767	0	нон	57	75.288	70.156	31.710		40.54		0
HETATM	2768	0	нон	58	64.697	73.440	32.795	1.00	34.94		Ο.
HETATM	2769	0	нон	59	66.251	37.651	16.856	1.00	33.53		0
HETATM	2770	0	НОН	60	63.282	31.611	25.681	1.00	44.64		0
HETATM	2771	0	нон	61	71.430	55.918	41.920		36.49		0
HETATM		0	НОН	62	65.638	58.677	21.385	1.00	35.26		0
HETATM	2773	0	НОН	63	55.080	46.995	17.425		53.19		0
HETATM	2774	0	НОН	64		31.766	16.460		43.10		0
HETATM	2775	0	НОН	65	74.644	37.157	10.791		39.58		0
HETATM	2776	0	HOH	66	62.315	61.756	37.610		36.98		0
HETATM	2777	0	HOH	67	73.617	64.778	30.740				0
HETATM	2778	0	HOH	68	55.753	71.270	16.210		37.70		0

HE	MTAT	2779	0	нон	69	60.894	73.990	38.995	1.00 52.68		0
HE	MTAT	2780	0	HOH	70	54.230	73.527	38.967	1.00 53.01		0
HE	MTAT	2781	0	HOH	71	85.347	49.247	39.609	1.00 46.03		0
HE	MTAT	2782	0	HOH	72	90.366	44.868	34.983	1.00 60.08		0
HE	MTAT	2783	0	HOH	73	74.553	34.802	40.308	1.00 42.36		0
HE	MTAT	2784	0	HOH	74	92.253	47.877	34.577	1.00 48.24		0
HE	MTAT	2785	0	HOH	75	62.333	64.301	35.516	1.00 42.55		0
HE	MTAT	2786	0	HOH	76	75.293	38.619	8.177	1.00 42.95		0
HE	MTAT	2787	0	HOH	77	74.834	47.737	35.645	1.00 45.47		0
ΗE	MTAT	2788	0	HOH	78	43.248	43.725	23.511	1.00 41.40		0
HE	MTAT	2789	0	HOH	79	92.749	48.847	23.299	1.00 48.74		0
ΗE	MTAT	2790	0	HOH	80	81.622	38.388	24.165	1.00 48.40		0
HE	MTAT	2791	0	HOH	81	69.535	35.845	7.684	1.00 44.93		0
HE	MTAT	2792	0	HOH	82	66.021	28.568	15.079	1.00 43.38		0
HE	MTAT	2793	0	HOH	83	63.363	58.444	43.595	1.00 60.19		0
HE	MTAT	2794	0	HOH	84	50.760	46.222	35.814	1.00 40.54		0
HE	MTAT	2795	0	HOH	85	73.050	33.188	26.343	1.00 59.24		0
HE	MTAT	2796	0	HOH	86	60.595	29.978	22.680	1.00 52.27		0
HE	MTAT	2797	0	HOH	87	69.555	45.175	46.108	1.00 47.35		0
HE	MTAT	2798	0	HOH	88	91.680	50.881	35.482	1.00 58.01		0
HE	MTAT	2799	0	НОН	- 89	54.754	33:372	37.626	1.00 47.38		0
HE	MTAT	2800	0	нон	90	70.270	53.925	17.757	1.00 43.71		0
HE	MTAT	2801	0	нон	91	86.174	38.632	29.884	1.00 51.68		0
HE	MTAT	2802	0	HOH	92	50.223	32.982	11.986	1.00 53.26		0
HE	MTAT	2803	0	нон	93	69.797	32.727	38.335	1.00 48.52		0
HE	MTAT	2804	0	нон	94	45.294	44.791	32.974	1.00 45.93		0
HE	MTAT	2805	0	HOH	95	50.957	50.719	21.814	1.00 47.04		0
HE	MTAT	2806	0	HOH	96	67.427	59.503	38.921	1.00 51.20		0
HE	MTAT	2807	0	нон	97	45.814	48.859	27.359	1.00 52.57		0
HE	MTAT	2808	0	нон	98	67.272	72.374	31.829	1.00 43.34		0
HE	MTAT	2809	0	нон	99	81.547	54.867	13.482	1.00 56.22		0
HE	MTAT	2810	0	нон	100	73.436	41.135	42.320	1.00 51.99		0
HE	MTAT	2811	0	HOH	101	45.438	41.435	12.889	1.00 51.81		0
HE	MTAT	2812	0	HOH	102	72.135	31.364	23.780	1.00 49.13		0
HE	MTAT	2813	0	нон	103	64.895	66.481	39.105	1.00 64.76		0
HE	MTAT	2814	Q	нон	104	67.577	69.286	38.086	1.00 45.89		0
ΗE	MTAT	2815	0	HOH	105	69.612	68.635	35.879	1.00 63.93		0
ΗE	MTAT	2816	0	HOH	106	72.031	67.254	32.046	1.00 48.47		0
HE	MTAT	2817	0	HOH	107	72.305	61.345	21.016	1.00 44.10		0
ΗE	MTAT	2818	0	HOH	108	74.756	62.694	19.263	1.00 48.65		0
HE	MTAT	2819	0.	HOH	109	95.910	46.347	27.675	1.00 53.29		0
ΗE	MTAT	2820	0	нон	110	94.046	48.897	25.977	1.00 51.23		0
ΗE	MTAT	2821	0	HOH	111	97.282	43.405	26.308	1.00 55.88		0
ΗE	MTAT	2822	0	HOH	112	96.131	51.037	25.453	1.00 43.15		0
HE	MTAT	2823	0	HOH	113	79.236	36.729	24.882	1.00 50.87		0
ΗE	MTAT	2824	0	HOH	114	79.234	40.387	31.965	1.00 38.53		0
HE	MTAT	2825	0	HOH	115	81.670	39.064	21.018	1.00 60.16	•	0
ΗE	MTAT	2826	0	HOH	116	60.063	41.314	40.014	1.00 53.39		0
ΗE	MTAT	2827	0	HOH	117	68.407	44.274	48.786	1.00 58.93		0
	MŢAT		0	HOH	118	73.852	38.881	40.464	1.00 54.08		0
	MTAT		0	HOH	119	66.435	34.694	36.949	1.00 50.41		0
	MTAT		0	HOH	120	68.667	31.549	25.842	1.00 64.44		0
	MTAT		0	нон	121	65.857	31.082	26.881	1.00 40.73		0
	MTAT		0	HOH	122	62.672	33.363	29.890	1.00 48.58		0
	MTAT		0	HOH	123	61.493	33.436	27.087	1.00 48.36		0
	MTAT		0	HOH	124	69.854	28.735	27.500	1.00 61.68		0
HE	MTAT	2835	0	HOH	125	64.874	31.147	29.825	1.00 60.07		0

```
HETATM 2836 O HOH 126 71.711 32.640 30.005 1.00 47.37 O
HETATM 2837 O HOH 127 52.466 50.282 19.032 1.00 52.65 O
HETATM 2838 O HOH 128 49.739 53.604 24.073 1.00 61.02 O
HETATM 2839 O HOH 129 48.481 31.684 25.480 1.00 54.44 O
HETATM 2840 O HOH 130 65.224 61.485 37.955 1.00 47.75 O
HETATM 2841 O HOH 131 72.681 36.196 7.328 1.00 60.10 O
HETATM 2842 O HOH 132 54.600 53.590 40.349 1.00 61.76 O
HETATM 2843 O HOH 133 55.212 44.260 39.797 1.00 54.33 O
HETATM 2844 O HOH 134 58.628 61.370 13.634 1.00 55.77 O
HETATM 2845 O HOH 135 78.074 50.966 38.251 1.00 55.68 O
HETATM 2846 O HOH 136 76.140 52.648 36.261 1.00 34.66 O
HETATM 2848 O HOH 138 74.079 55.395 38.640 1.00 55.76 O
HETATM 2849 O HOH 139 72.037 53.724 43.983 1.00 49.73 O
HETATM 2850 O HOH 140 89.745 53.305 35.869 1.00 47.56 O
HETATM 2851 O HOH 141 66.701 41.042 2.783 1.00 58.40 O
HETATM 2852 O HOH 142 92.676 53.997 36.233 1.00 50.74 O
HETATM 2855 O HOH 144 68.797 43.869 0.416 1.00 57.30 O
HETATM 2855 O HOH 144 68.797 43.869 0.416 1.00 57.30 O
HETATM 2855 O HOH 144 68.797 43.869 0.416 1.00 57.30 O
HETATM 2855 O HOH 144 68.797 43.869 0.416 1.00 57.30 O
 CONECT 202 2514
  CONECT 1501 1502
  CONECT 1502 1501 1503 1505
  CONECT 1503 1502 1504
  CONECT 1504 1503 1507
  CONECT 1505 1502 1506
  CONECT 1506 1505
  CONECT 1507 1504
  CONECT 2514 202
  CONECT 2688 2689 2690 2691 2692
  CONECT 2689 2688
  CONECT 2690 2688
  CONECT 2691 2688
  CONECT 2692 2688 2693
  CONECT 2693 2692 2694
  CONECT 2694 2693 2695 2696
  CONECT 2695 2694 2700
  CONECT 2696 2694 2697 2698
  CONECT 2697 2696
  CONECT 2698 2696 2699 2700
  CONECT 2699 2698
  CONECT 2700 2695 2698 2701
  CONECT 2701 2700 2702 2710
  CONECT 2702 2701 2703
 CONECT 2703 2702 2704
 CONECT 2704 2703 2705 2710
 CONECT 2705 2704 2706 2707
  CONECT 2706 2705
  CONECT 2707 2705 2708
  CONECT 2708 2707 2709
  CONECT 2709 2708 2710
  CONECT 2710 2701 2704 2709
 MASTER 521 0 3 14
                                                                        18
                                                                                      0
                                                                                           0
                                                                                                           6 2854 1 32
                                                                                                                                                    39
 END
 Figure 11
  P-UC 5440
 Page 1
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```
HEADER
         OXIDOREDUCTASE
                                                08-AUG-02
                                                           1MEH
         INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
TITLE
TITLE
        2 TRITRICHOMONAS FOETUS WITH IMP AND MOA BOUND
COMPND
        MOL ID: 1;
COMPND
        2 MOLECULE: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE;
COMPND 3 CHAIN: A;
COMPND 4 SYNONYM: IMP DEHYDROGENASE, IMPDH;
COMPND
        5 EC: 1.1.1.205;
COMPND 6 ENGINEERED: YES
SOURCE
        MOL ID: 1;
SOURCE
        2 ORGANISM SCIENTIFIC: TRITRICHOMONAS FOETUS;
SOURCE 3 GENE: IMPDH;
SOURCE 4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE 5 EXPRESSION SYSTEM COMMON: BACTERIA;
SOURCE 6 EXPRESSION SYSTEM STRAIN: H712;
SOURCE 7 EXPRESSION SYSTEM VECTOR TYPE: PLASMID;
SOURCE 8 EXPRESSION SYSTEM PLASMID: PBACE
KEYWDS ALPHA BETA BARREL
EXPDTA
       X-RAY DIFFRACTION
AUTHOR
         G.L. PROSISE, H. LUECKE
JRNL
           AUTH
                  G.L. PROSISE, H. LUECKE
JRNL
           TITL
                  CRYSTAL STRUCTURE OF T. FOETUS INOSINE
           TITL 2 MONOPHOSPHATE DEHYDROGENASE IN COMPLEX WITH
JRNL
JRNL
           TITL 3 SUBSTRATE, COFACTOR, AND ANALOGS:STRUCTURAL BASIS
          TITL 4 FOR THE RANDOM-IN ORDERED-OUT KINETIC MECHANISM
JRNL
JRNL
           REF
                  TO BE PUBLISHED
           REFN
JRNL
REMARK
        1
REMARK
REMARK 2 RESOLUTION. 1.95 ANGSTROMS.
REMARK 3
REMARK 3 REFINEMENT.
REMARK 3 PROGRAM
                       : CNS 1.1
                       : BRUNGER, ADAMS, CLORE, DELANO, GROS, GROSSE-
REMARK 3
            AUTHORS
REMARK 3
                        : KUNSTLEVE, JIANG, KUSZEWSKI, NILGES, PANNU,
REMARK 3
                        : READ, RICE, SIMONSON, WARREN
REMARK 3
REMARK
        3 REFINEMENT TARGET : ENGH & HUBER
REMARK
REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 1.95
REMARK 3
            RESOLUTION RANGE LOW (ANGSTROMS): 19.98
REMARK 3
            DATA CUTOFF
                                  (SIGMA(F)) : 0.000
            OUTLIER CUTOFF HIGH (RMS (ABS (F))) : NULL
REMARK 3
REMARK 3
            COMPLETENESS (WORKING+TEST) (%): 98.6
REMARK 3
            NUMBER OF REFLECTIONS
                                             : 44863
REMARK
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3
           CROSS-VALIDATION METHOD
                                           : THROUGHOUT
REMARK 3
            FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE
                              (WORKING SET) : 0.243
REMARK 3 FREE R VALUE
REMARK 3 FREE R VALUE TEST SET SIZE
                                        (%): 5.100
REMARK 3
            FREE R VALUE TEST SET COUNT
                                            : 2294
REMARK 3
            ESTIMATED ERROR OF FREE R VALUE : 0.006
REMARK
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
```

```
REMARK 3 TOTAL NUMBER OF BINS USED
                                            : 6
REMARK 3 BIN RESOLUTION RANGE HIGH
REMARK 3 BIN RESOLUTION RANGE LOW
                                       (A) : 1.95
                                     (A) : 2.07
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 96.70
REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 6852
REMARK 3 BIN R VALUE (WORKING SET) : 0.26
                               (WORKING SET) : 0.2630
REMARK 3 BIN FREE R VALUE
                                       : 0.2960
REMARK 3 BIN FREE R VALUE TEST SET SIZE (%) : 4.60
REMARK 3 BIN FREE R VALUE TEST SET COUNT : 333
REMARK 3
            ESTIMATED ERROR OF BIN FREE R VALUE : 0.016
REMARK
        3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 2709
REMARK 3 NUCLEIC ACID ATOMS
                                 : 0
REMARK 3 HETEROGEN ATOMS
                                  : 47
                               : 4,
: 193
REMARK 3 SOLVENT ATOMS
REMARK
        3
      3 B VALUES.
REMARK
REMARK 3 FROM WILSON PLOT (A**2): 19.90
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 32.70
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : 0.00000
REMARK 3 B22 (A**2) : 0.00000
REMARK 3 B33 (A**2) : 0.00000
REMARK 3 B12 (A**2) : 0.00000
REMARK 3
REMARK 3 B23 (A**2) : 0.00000
REMARK 3
           B13 (A**2) : 0.00000
REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM LUZZATI PLOT
                                      (A) : 0.25
REMARK 3 ESD FROM SIGMAA
                                      (A) : 0.15
REMARK 3 LOW RESOLUTION CUTOFF
                                     (A) : 5.00
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT (A): 0.29
REMARK 3 ESD FROM C-V SIGMAA
                                     (A) : 0.18
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS
                                      (A): 0.006
REMARK 3 BOND ANGLES
                                (DEGREES) : 1.20
REMARK 3 DIHEDRAL ANGLES (DEGREES): 22.30
REMARK 3 IMPROPER ANGLES (DEGREES): 0.70
REMARK
        3
REMARK 3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                              RMS
REMARK
        3 MAIN-CHAIN BOND (A**2): 0.810; 1.500
REMARK
        3 MAIN-CHAIN ANGLE
                                     (A**2) : 1.440 ; 2.000
                                (A**2) : 1.060 ; 2.000
REMARK
        3 SIDE-CHAIN BOND
REMARK
          SIDE-CHAIN ANGLE
                                      (A**2) : 1.700 ; 2.500
REMARK 3
REMARK 3 BULK SOLVENT MODELING.
REMARK 3 METHOD USED : FLAT MODEL
REMARK 3 KSOL : 0.40
REMARK 3 BSOL
                     : 48.93
REMARK 3
REMARK 3 NCS MODEL : NULL
```

```
REMARK 3
REMARK 3 NCS RESTRAINTS.
                                                RMS SIGMA/WEIGHT
REMARK 3 GROUP 1 POSITIONAL (A): NULL ; NULL REMARK 3 GROUP 1 B-FACTOR (A**2): NULL ; NULL
REMARK 3
REMARK 3 PARAMETER FILE 1 : PROTEIN REP.PARAM
REMARK 3 PARAMETER FILE 2 : PARAM.GNSOL
REMARK 3 PARAMETER FILE 3 : CIS_PEPTIDE.PARAM
REMARK 3 PARAMETER FILE 4 : MPA.PAR
REMARK 3 PARAMETER FILE 5 : IMP.PAR
REMARK 3 PARAMETER FILE 6 : NULL
REMARK 3 TOPOLOGY FILE 1 : PROTEIN.TOP
REMARK 3 TOPOLOGY FILE 2 : IMP.TOP
REMARK 3 TOPOLOGY FILE 3 : MPA.TOP
REMARK 3 TOPOLOGY FILE 4 : K.TOP
REMARK 3 TOPOLOGY FILE 5 : TOPH.GNSOL
REMARK 3 TOPOLOGY FILE 6 : NULL
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: NULL
REMARK 4
REMARK 4 1MEH COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 16-AUG-2002.
REMARK 100 THE RCSB ID CODE IS RCSB016852.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION REMARK 200 DATE OF DATA COLLECTION : 11-APR-2001
REMARK 200 TEMPERATURE (KELVIN) : 100.0
REMARK 200 PH
                                     : 7.50
REMARK 200 NUMBER OF CRYSTALS USED
                                        : 1
REMARK 200
REMARK 200 SYNCHROTRON
REMARK 200 SYNCHROTRON (Y/N): Y
REMARK 200 RADIATION SOURCE : SSRL
REMARK 200 BEAMLINE
                                        : 9-1
                                   : NULL
REMARK 200 X-RAY GENERATOR MODEL : NURSEMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE
                                  (A) : 0.97
REMARK 200 MONOCHROMATOR
                                        : NULL
REMARK 200 OPTICS
                                        : NULL
REMARK 200
           .
REMARK 200 DETECTOR TYPE
REMARK 200 DETECTOR TYPE : IMAGE PLATE REMARK 200 DETECTOR MANUFACTURER : MARRESEARCH
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE
                                        : SCALEPACK
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 44997
REMARK 200 RESOLUTION RANGE HIGH (A): 1.950
REMARK 200 RESOLUTION RANGE LOW (A) : 20.000
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NULL
REMARK 200
REMARK 200 OVERALL.
                                   (%): 99.0
REMARK 200 COMPLETENESS FOR RANGE
REMARK 200 DATA REDUNDANCY
                                     : 5.400
(I) : 0.05700
REMARK 200 R MERGE
                                  (I) : NULL
REMARK 200 R SYM
REMARK 200 <I/SIGMA(I) > FOR THE DATA SET : 25.9000
```

```
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 1.95
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : 1.98
REMARK 200 COMPLETENESS FOR SHELL (%): 95.7
REMARK 200 DATA REDUNDANCY IN SHELL : NULL
REMARK 200 R MERGE FOR SHELL (I)

**TOTOMA(T) > FOR SHELL (I)
REMARK 200 R MERGE FOR SHELL (I): 0.66000
                                        (I) : NULL
                                              : 1.820
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: FOURIER SYNTHESIS
REMARK 200 SOFTWARE USED: CNS
REMARK 200 STARTING MODEL: PDB ENTRY 1AK5
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: SODIUM MALONATE, TRIS, 2-
REMARK 280 MERCAPTOETHANOL, EDTA, GLYCEROL
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 4 3 2
REMARK 290
REMARK 290
               SYMOP SYMMETRY
REMARK 290
              NNNMMM OPERATOR
REMARK 290
               1555 X,Y,Z
REMARK 290
              2555 -X,-Y,Z
              3555
REMARK 290
                         -X,Y,-Z
             4555 X,-Y,-Z
REMARK 290
REMARK 290 5555 Z,X,Y

REMARK 290 6555 Z,-X,-Y

REMARK 290 7555 -Z,-X,Y

REMARK 290 8555 -Z,X,-Y

REMARK 290 9555 Y,Z,X

REMARK 290 10555 -Y,Z,-X
REMARK 290 11555 Y,-Z,-X
REMARK 290 12555 -Y,-Z,X
REMARK 290 13555 Y,X,-Z
REMARK 290 14555 -Y,-X,-Z
REMARK 290 15555 Y,-X,Z
REMARK 290 16555 -Y,X,Z
REMARK 290
               17555 X,Z,-Y
               18555 -X,Z,Y
REMARK 290
               19555
REMARK 290
                         -X,-Z,-Y
               20555 X,-Z,Y
REMARK 290
               21555
                        Z,Y,-X
REMARK 290
REMARK 290
               22555
                        Z,-Y,X
REMARK 290
               23555 -Z,Y,X
REMARK 290
               24555 -Z,-Y,-X
REMARK 290
REMARK 290 WHERE NNN -> OPERATOR NUMBER
              MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290
```

TABLE 3

REMARK						TRY TRANSFO		
REMARK								ATOM/HETATM
REMARK		RECORDS I				ro produce	CRYSTALLOGR	APHICALLY
REMARK		RELATED N						
REMARK		SMTRY1	1		000000	0.000000	0.000000	0.00000
REMARK		SMTRY2	1		000000	1.000000	0.00000	0.00000
REMARK		SMTRY3	1		000000	0.00000	1.000000	0.00000
REMARK		SMTRY1	2		000000	0.000000	0.000000	0.00000
REMARK		SMTRY2	2		000000	-1.000000	0.000000	0.00000
REMARK		SMTRY3	2		000000	0.000000	1.000000	0.00000
REMARK		SMTRY1	3		000000	0.000000	0.000000	0.00000
REMARK		SMTRY2	3		000000	1.000000	0.000000	0.00000
REMARK		SMTRY3	3		000000	0.000000	-1.000000	0.00000
REMARK		SMTRY1	4		000000	0.000000	0.000000	0.00000
REMARK		SMTRY2	4		.000000	-1.000000	0.000000	0.00000
REMARK		SMTRY3	4		.000000	0.000000	-1.000000	0.00000
REMARK		SMTRY1	5		.000000	0.000000	1.000000	0.00000
REMARK		SMTRY2	5		.000000	0.000000	0.000000	0.00000
REMARK		SMTRY3	- 5		.000000	1.000000	0.000000	0.00000
REMARK		SMTRY1	6		.000000	0.000000	1.000000	0.00000
REMARK		SMTRY2	6		.000000	0.000000	0.000000	0.00000
REMARK		SMTRY3	6		.000000		0.000000	0.00000
REMARK		SMTRY1	7		. 000000	0.000000	-1.000000	0.00000
REMARK		SMTRY2	7		. 000000		0.000000	0.00000
REMARK		SMTRY3	7		. 000000		0.000000 -1.000000	0.00000
REMARK		SMTRY1	8		.000000 .000000		0.000000	0.00000
REMARK REMARK		SMTRY2 SMTRY3	8 8		. 000000 . 000000		0.000000	0.00000
REMARK		SMTRY1	9		. 000000 . 000000	1.000000	0.000000	0.00000
REMARK		SMTRY2	. 9		. 000000		1.000000	0.00000
REMARK		SMTRY3	9		. 000000		0.000000	0.00000
REMARK		SMTRY1	10		. 000000		0.000000	0.00000
REMARK		SMTRY2	10		.000000		1.000000	0.00000
REMARK		SMTRY3	10		.000000		0.000000	0.00000
REMARK		SMTRY1	11		. 000000		0.00000	0.00000
REMARK		SMTRY2	11	0	. 000000	0.000000	-1.000000	0.00000
REMARK		SMTRY3	11	-1	. 000000	0.000000	0.00000	0.00000
REMARK	290	SMTRY1	12	0	.000000	-1.000000	0.00000	. 0.00000
REMARK	290	SMTRY2	12	0	.000000	0.000000	-1.000000	0.00000
REMARK	290	SMTRY3	12	1	.000000	0.000000	0.00000	0.00000
REMARK	290	SMTRY1	13	0	.000000	1.000000	0.00000	0.00000
REMARK	290	SMTRY2	13	1	.000000	0.000000	0.00000	0.00000
REMARK	290	SMTRY3	13	0	.000000	0.00000		0.00000
REMARK	290	SMTRY1	14	0	.000000		0.00000	0.00000
REMARK	290	SMTRY2	14		.000000		0.00000	0.00000
REMARK		SMTRY3	14		.000000			0.00000
REMARK		SMTRY1			. 000000		0.00000	0.00000
REMARK		SMTRY2	15		. 000000		0.00000	0.00000
REMARK			15		.000000		1.000000	0.00000
REMARK		SMTRY1			.000000		0.000000	0.00000
REMARK		SMTRY2			.000000		0.000000	0.00000
REMARK		SMTRY3			.000000		1.000000	0.00000
REMARK		SMTRY1			.000000		0.000000	0.00000
REMARK		SMTRY2			.000000		1.000000	0.00000
REMARK		SMTRY3			.000000		0.000000	0.00000 0.00000
REMARK		SMTRY1			.000000		0.000000	0.00000
REMARK	290	SMTRY2	18	U	.000000	0.000000	1.000000	0.0000

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```
REMARK 290 SMTRY3 18 0.000000 1.000000 0.000000
                                                                          0.00000
REMARK 290 SMTRY1 19 -1.000000 0.000000 0.000000 REMARK 290 SMTRY2 19 0.000000 0.000000 -1.000000 REMARK 290 SMTRY3 19 0.000000 -1.000000 0.000000
                                                                           0.00000
                                                                           0.00000
REMARK 290 SMTRY3 19 0.000000 -1.000000 0.000000 REMARK 290 SMTRY1 20 1.000000 0.000000 -1.000000 0.000000 REMARK 290 SMTRY2 20 0.000000 0.000000 -1.000000 REMARK 290 SMTRY3 20 0.000000 1.000000 0.000000 REMARK 290 SMTRY1 21 0.000000 0.000000 1.000000 REMARK 290 SMTRY2 21 0.000000 1.000000 0.000000 REMARK 290 SMTRY3 21 -1.000000 0.000000 0.000000 REMARK 290 SMTRY3 21 -1.000000 0.000000 0.000000 REMARK 290 SMTRY3 21 -1.000000 0.000000 0.000000 REMARK 290 SMTRY3 22 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 22 0.000000 0.000000 0.000000 0.000000
                                                                          0.00000
                                                                          0.00000
                                                                          0.00000
                                                                          0.00000
                                                                          0.00000
                                                                          0.00000
                                                                          0.00000
REMARK 290 SMTRY2 22 0.000000 -1.000000 0.000000
                                                                          0.00000
REMARK 290 SMTRY3 22 1.000000 0.000000 0.000000
REMARK 290 SMTRY1 23 0.000000 0.000000 -1.000000
                                                                          0.00000
REMARK 290 SMTRY2 23 0.000000 1.000000 0.000000
                                                                          0.00000
REMARK 290 SMTRY3 23 1.000000 0.000000 0.000000
                                                                           0.00000
REMARK 290 SMTRY1 24 0.000000 0.000000 0.000000 REMARK 290 SMTRY2 24 0.000000 -1.000000 0.000000 REMARK 290 SMTRY3 24 -1.000000 0.000000 0.000000
                                                                           0.00000
                                                                          0.00000
                                                                          0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 1 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW: BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000
                                                                          0.00000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000
                                                                           0.00000
REMARK 350 BIOMT3 3 0.000000 0.000000 1.000000
                                                                           0.00000
REMARK 350 BIOMT1 4 0.000000 -1.000000 0.000000
                                                                       153.48000
REMARK 350 BIOMT2 4 1.000000 0.000000 0.000000
                                                                          0.00000
              BIOMT3 4 0.000000 0.000000 1.000000
REMARK 350
                                                                           0.00000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465 M RES C SSSEQI
REMARK 465 MET A 1
REMARK 465 ASP A 107
```

REMARK	465	SER A	108
REMARK	465	ASN A	109
REMARK	465	VAL A	110
REMARK	465	LYS A	111
REMARK	465	PRO A	112
REMARK	465	ASP A	113
REMARK	465	GLN A	114
REMARK	465	THR A	115
REMARK	465	PHE A	116
REMARK	465	ALA A	117
REMARK	465	ASP A	118
REMARK	465	VAL A	119
REMARK	465	LEU A	120
REMARK	465	ALA A	121
REMARK	465	ILE A	122
REMARK	465	SER A	123
REMARK	465	GLN A	124
REMARK	465	ARG A	125
REMARK	465	THR A	126
REMARK	465	THR A	127
REMARK	465	HIS A	128
REMARK	465	ASN A	129
REMARK	465	THR A	130
REMARK	465	VAL A	131
REMARK	465	ALA A	132
REMARK	465	VAL A	133
REMARK	465	THR A	134
REMARK	465	ASP A	135
REMARK	465	ASP A	136
REMARK	465	GLY A	137
REMARK	465	THR A	138
REMARK	465	PRO A	139
REMARK.	465	HIS A	140
REMARK	465	GLY A	141
REMARK	465	VAL A	142
REMARK	465	LEU A	143
REMARK	465	LEU A	144
REMARK	465	GLY A	145
REMARK	465	LEU A	146
REMARK	465	VAL A	147
REMARK	465	THR A	148
REMARK	465	GLN A	149
REMARK	465	ARG A	150
REMARK	465	ASP A	151
REMARK	465	TYR A	152
REMARK	465	PRO A	153
	465	ILE A	154
	465	ASP A	155
	465	LEU A	156
	465	THR A	157
	465	GLN A	158
REMARK		THR A	159
REMARK		GLU A	160
REMARK		THR A	161
	465	LYS A	162
	465	VAL A	163
REMARK	465	SER A	164

REMARK 465	ASP A	165
REMARK 465	MET A	166
REMARK 465	MET A	167
REMARK 465	THR A	168
REMARK 465	PRO A	169
REMARK 465	PHE A	170
REMARK 465	SER A	171
REMARK 465	LYS A	172
REMARK 465	LEU A	173
REMARK 465	VAL A	174
REMARK 465	THR A	175
REMARK 465	ALA A	176
REMARK 465	HIS A	177
REMARK 465	GLN A	178
REMARK 465	ASP A	179
REMARK 465	THR A	180
REMARK 465	LYS A	181
REMARK 465	LEU A	182
REMARK 465	SER A	183
REMARK 465	GLU A	184
REMARK. 465	ALA A	185
REMARK 465	ASN A	186
REMARK 465	LYS A	187
REMARK 465	ILE A	188
REMARK 465	ILE A	189
REMARK 465	TRP A	190
REMARK 465	GLU A	191
REMARK 465	LYS A	192
REMARK 465	LYS A	193
REMARK 465	LEU A	194
REMARK 465	ASN A	195
REMARK 465	ALA A	196
	LEU A	197
REMARK 465 REMARK 465	PRO A	198
	ILE A	199
REMARK 465	ILE A	200
REMARK 465		201
REMARK 465	ASP A ASP A	201
REMARK 465	ASP A	202
REMARK 465 REMARK 465	GLN A	203
		204
REMARK 465		203
REMARK 465		207
REMARK 465		207
REMARK 465	TYR A	
REMARK 465	ILE A	209
REMARK 465	VAL A	210
REMARK 465	PHE A	211
REMARK 465	ARG A	212
REMARK 465	LYS A	213
REMARK 465	ASP A	214
REMARK 465	TYR A	215
REMARK 465	ASP A	216
REMARK 465	ARG A	217
REMARK 465	SER A	218
REMARK 465	GLN A	219
REMARK 465	VAL A	220
REMARK 465	CYS A	221

TABLE 3 125 .

```
REMARK 465
             GLN A
            ARG A 418
REMARK 465
REMARK 465
            TYR A 419
REMARK 465
            ASP A 420
REMARK 465
            LEU A 421
                    422
REMARK 465
            GLY A
            GLY A
REMARK 465
                     423
            LYS A
REMARK 465
                     424
            GLN A
REMARK 465
                     425
REMARK 465
            LYS A 426
REMARK 465
            LEU A 427
REMARK 465
            SER A 428
REMARK 465
            PHE A 429
             VAL A 484
REMARK 465
             GLU A 485
REMARK 465
REMARK 465
            GLY A
                    486
REMARK 465
            GLY A 487
REMARK 465
            ALA A 488
REMARK 465
            HIS A 489
REMARK 465
            ASP A
                     490
REMARK 465 VAL A 491
                    492
             ILE A
REMARK 465
             VAL A
                     493
REMARK 465
            LYS A 494
REMARK 465
            ASP A 495
REMARK 465
REMARK 465
            ARG A 496
REMARK 465
            ILE A 497
REMARK 465
            ASN A 498
REMARK 465
            ASP A 499
REMARK 465
              TYR A 500
REMARK 465
             HIS A
                     501
REMARK 465 PRO A
                     502
REMARK 465
              LYS A 503
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, 2(A3, 1X, A1, I4, A1, 1X, A4, 3X), F6.3)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
                                              DEVIATION
REMARK 500 M RES CSSEQI ATM1
                              RES CSSEOI ATM2
REMARK 500 PRO A 354 CG
                              PRO A 354 CB
                                               0.033
                                                0.035
REMARK 500
             MET A 373
                        CE
                              MET A 373
                                         SD
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
```

```
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1
                               ATM2
                                      ATM3
REMARK 500
             GLY A 20
                         N
                             - CA
                                      C
                                          ANGL. DEV. = -8.3 DEGREES
REMARK 500
             ILE A
                    27
                         N
                               CA
                                       C
                                          ANGL. DEV. = -8.2 DEGREES
                             - CA
                                   _
REMARK 500
            GLN A 45
                         N
                                      C
                                          ANGL. DEV. = -8.3 DEGREES
                         N · - CA -
           ILE A 52
                                          ANGL. DEV. = -7.8 DEGREES
REMARK 500
                                      С
                           - CA -
REMARK 500
           PRO A 53
                         N
                                      C
                                          ANGL. DEV. = 7.0 DEGREES
                           - CA - C
                                         ANGL. DEV. = 8.6 DEGREES
REMARK 500
           SER A 63
                         N
REMARK 500
           PHE A 266
                            - CA - C
                                          ANGL. DEV. = -8.1 DEGREES
                         N
                             - CA -
                                          ANGL. DEV. = -7.7 DEGREES
REMARK 500
             LYS A 394
                                      C
                         N
                                          ANGL. DEV. = 7.3 DEGREES
                            - CA -
REMARK 500
             LYS A 472
                         N
                                      С
                                          ANGL. DEV. = -8.1 DEGREES
REMARK 500
             LYS A 474
                         N
                            - CA -
                                      C
                         :N - CA -
                                      С
                                          ANGL. DEV. = -7.0 DEGREES
REMARK 500
            LEU A 477
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1AK5
                             RELATED DB: PDB
REMARK 900 INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
REMARK 900 TRITRICHOMONAS FOETUS
REMARK 900 RELATED ID: 1ME7
                            RELATED DB: PDB
REMARK 900 1ME7 CONTAINS THE SAME PROTEIN WITH RVP AND MOA BOUND
REMARK 900 RELATED ID: 1ME8
                            RELATED DB: PDB
REMARK 900 1ME8 CONTAINS THE SAME PROTEIN WITH RVP BOUND
REMARK 900 RELATED ID: 1ME9
                            RELATED DB: PDB
REMARK 900 1ME9 CONTAINS THE SAME PROTEIN WITH IMP BOUND
REMARK 900 RELATED ID: 1MEI
                           RELATED DB: PDB
REMARK 900 1MEI CONTAINS THE SAME PROTEIN WITH XMP AND MYCOPHENOLIC
REMARK 900 ACID BOUND
REMARK 900 RELATED ID: 1MEW
                            RELATED DB: PDB
REMARK 900 1MEW CONTAINS THE SAME PROTEIN WITH XMP AND NAD BOUND
                                         IMDH TRIFO
DBREF 1MEH A
                1
                    503 SWS
                                P50097
                                                              503
SEQADV 1MEH CSO A 319 SWS P50097
                                           319 MODIFIED RESIDUE
                                     CYS
        1 A 503 MET ALA LYS TYR TYR ASN GLU PRO CYS HIS THR PHE ASN
SEQRES
                 GLU TYR LEU LEU ILE PRO GLY LEU SER THR VAL ASP CYS
SEQRES
        2 A 503
                  ILE PRO SER ASN VAL ASN LEU SER THR PRO LEU VAL LYS
SEQRES
        3 A 503
SEQRES
        4 A 503 PHE GLN LYS GLY GLN GLN SER GLU ILE ASN LEU LYS ILE
SEQRES
       5 A 503 PRO LEU VAL SER ALA ILE MET GLN SER VAL SER GLY GLU
SEQRES 6 A 503 LYS MET ALA ILE ALA LEU ALA ARG GLU GLY GLY ILE SER
SEQRES 7 A 503 PHE ILE PHE GLY SER GLN SER ILE GLU SER GLN ALA ALA
SEQRES 8 A 503 MET VAL HIS ALA VAL LYS ASN PHE LYS ALA GLY PHE VAL
SEQRES
       9 A 503 VAL SER ASP SER ASN VAL LYS PRO ASP GLN THR PHE ALA
SEQRES 10 A 503 ASP VAL LEU ALA ILE SER GLN ARG THR THR HIS ASN THR
SEORES 11 A 503
                 VAL ALA VAL THR ASP ASP GLY THR PRO HIS GLY VAL LEU
SEQRES 12 A 503 LEU GLY LEU VAL THR GLN ARG ASP TYR PRO ILE ASP LEU
SEQRES 13 A 503 THR GLN THR GLU THR LYS VAL SER ASP MET MET THR PRO
SEQRES 14 A 503 PHE SER LYS LEU VAL THR ALA HIS GLN ASP THR LYS LEU
SEQRES 15 A 503 SER GLU ALA ASN LYS ILE ILE TRP GLU LYS LYS LEU ASN
SEQRES 16 A 503 ALA LEU PRO ILE ILE ASP ASP GLN HIS LEU ARG TYR
SEQRES 17 A 503 ILE VAL PHE ARG LYS ASP TYR ASP ARG SER GLN VAL CYS
SEQRES 18 A 503 HIS ASN GLU LEU VAL ASP SER GLN LYS ARG TYR LEU VAL
SEQRES 19 A
             503
                  GLY ALA GLY ILE ASN THR ARG ASP PHE ARG GLU ARG VAL
SEORES 20 A
             503 PRO ALA LEU VAL GLU ALA GLY ALA ASP VAL LEU CYS ILE
```

```
ASP SER SER ASP GLY PHE SER GLU TRP GLN LYS ILE THR
SEORES 21 A 503
                 ILE GLY TRP ILE ARG GLU LYS TYR GLY ASP LYS VAL LYS
SEQRES 22 A 503
SEORES 23 A 503 VAL GLY ALA GLY ASN ILE VAL ASP GLY GLU GLY PHE ARG
SEQRES 24 A 503 TYR LEU ALA ASP ALA GLY ALA ASP PHE ILE LYS ILE GLY
SEORES 25 A 503 ILE GLY GLY GLY SER ILE CSO ILE THR ARG GLU GLN LYS
SEQRES 26 A 503 GLY ILE GLY ARG GLY GLN ALA THR ALA VAL ILE ASP VAL
                 VAL ALA GLU ARG ASN LYS TYR PHE GLU GLU THR GLY ILE
SEQRES 27 A 503
                  TYR ILE PRO VAL CYS SER ASP GLY GLY ILE VAL TYR ASP
SEQRES 28 A 503
SEQRES 29 A 503 TYR HIS MET THR LEU ALA LEU ALA MET GLY ALA ASP PHE
SEORES 30 A 503 ILE MET LEU GLY ARG TYR PHE ALA ARG PHE GLU GLU SER
SEQRES 31 A 503 PRO THR ARG LYS VAL THR ILE ASN GLY SER VAL MET LYS
SEQRES 32 A 503 GLU TYR TRP GLY GLU GLY SER SER ARG ALA ARG ASN TRP
SEQRES 33 A. 503 GLN ARG TYR ASP LEU GLY GLY LYS GLN LYS LEU SER PHE
SEORES 34 A 503 GLU GLU GLY VAL ASP SER TYR VAL PRO TYR ALA GLY LYS
SEQRES 35 A 503 LEU LYS ASP ASN VAL GLU ALA SER LEU ASN LYS VAL LYS
SEQRES 36 A 503 SER THR MET CYS ASN CYS GLY ALA LEU THR ILE PRO GLN
SEQRES 37 A 503 LEU GLN SER LYS ALA LYS ILE THR LEU VAL SER SER VAL
SEQRES 38 A 503 SER ILE VAL GLU GLY GLY ALA HIS ASP VAL ILE VAL LYS
SEQRES 39 A 503 ASP ARG ILE ASN ASP TYR HIS PRO LYS
MODRES 1MEH CSO A 319 CYS S-HYDROXYCYSTEINE
       CSO A 319
                       7
HET
       K A 900
HET
                      1
       IMP 602
HET
                      23
           600
HET
       MOA
                      23
       CSO S-HYDROXYCYSTEINE
HETNAM
           K POTASSIUM ION
HETNAM
          IMP INOSINIC ACID
HETNAM
        MOA MYCOPHENOLIC ACID
HETNAM
          MOA 6-(1,3-DIHYDRO-7-HYDROXY-5-METHOXY-4-METHYL-1-
HETSYN
HETSYN 2 MOA OXOISOBENZOFURAN-6-YL)-4-METHYL-4-HEXANOIC ACID
FORMUL 1 CSO
                C3 H7 N1 O3 S1
FORMUL 2 K
                  K1 1+
FORMUL 3 IMP
                  C10 H13 N4 O8 P1
FORMUL 4 MOA
                  C17 H20 O6
FORMUL
        5 HOH
                 *193(H2 O1)
                                                                       3
           1 THR A
                      11 ASN A
                                 13 5
HELIX
         1
                                                                       5
           2 ILE A
                      27
                         VAL A
                                 31
HELIX
         2
                         GLU A 74
                                                                      11
            3 GLY A
                      64
                                     1
HELIX
         3
HELIX .
                                                                      14
           4 SER A
                     85
                         ASN A 98
                                     1
        4
                                                                      13
         5
           5 ASP A 242
                         GLY A 254 1
HELIX
                                                                      16
            6 SER A 267
                         GLY A 282 1
HELIX
         6
                                                                       3
            7 ASP A 283 VAL A 285 5
HELIX
         7
                                                                      12
            8 ASP A 294 GLY A 305 1
HELIX
         8
            9 GLY A 316 ARG A 322 5
                                                                      7
HELIX
        9
                                                                      21
            10 GLY A 330 GLY A 350 1
 HELIX
        10
            11 TYR A 363 MET A 373 1
                                                                      11
 HELIX
        11
                                                                       6
 HELIX
        12
           12 GLY A 381 ARG A 386 1
                                                                      20
 HELIX
        13 13 LYS A 442
                         CYS A 461
                                    1
                                                                       9
 HELIX
        14
           14 THR A 465 ALA A 473
                                     1
 SHEET
         1
            A 2 TYR A 15 LEU A 17
                                    0
                                                      N LEU A
            A 2 ILE A 475 LEU A 477 -1
 SHEET
         2
                                          THR A 476
             B 2 THR A 35
                          PRO A 36 0
 SHEET
         1
                                                         THR A
                           LEU A
                                 50 -1
                                       O LEU A 50
                                                      N
                                                               35
 SHEET
         2
             B 2 ASN A 49
 SHEET
         1
             C 2 PHE A 40
                           GLN A 41
                                     0
                                        O TYR A 352
                                                      N
                                                         PHE A
                                                                40
 SHEET
         2
             C 2 ILE A 351
                           TYR A 352 -1
             D 9 LEU A 54
                          SER A 56
                                    0
 SHEET
         1
                                                      N SER A
                          ILE A 80 1 O ILE A 77
 SHEET
             D 9 ILE A 77
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3 D 9 GLY A 235 ILE A 238 1 O GLY A 237 N ILE A 80
 SHEET
                 D 9 VAL A 257 ILE A 260 1 O CYS A 259
                                                                          N ILE A 238
 SHEET
             4
                D 9 VAL A 287 ILE A 292 1 O GLY A 288
 SHEET
             5
                                                                           N LEU A 258
 SHEET
                D 9 ILE A 309 ILE A 311 1 O LYS A 310
             6
                                                                          N ALA A 289
 SHEET
             7
                D 9 VAL A 355 ASP A 358 1 O CYS A 356
                                                                          N ILE A 311
 SHEET
             8 D 9 PHE A 377 LEU A 380 1 O MET A 379
                                                                            N SER A 357
 SHEET
             9 D 9 LEU A 54 SER A 56 1 N VAL A 55
                                                                            O ILE A 378
               E 3 LYS A 394 ILE A 397 0
 SHEET
             1
                E 3 SER A 400 TRP A 406 -1 O MET A 402
E 3 ASP A 434 PRO A 438 -1 O SER A 435
 SHEET
             2
                                                                            N VAL A 395
                                                                          N TYR A 405
 SHEET
             3
           1 CYS A 26 CYS A 459
1 GLY A 290 ASN A 291 0 1.32
 SSBOND
 CISPEP
 CRYST1 153.480 153.480 153.480 90.00 90.00 P 4 3 2
            1.000000 0.000000 0.000000 0.00000
 ORIGX1
                0.000000 1.000000 0.000000
                                                               0.00000
 ORIGX2
              0.000000 0.000000 1.000000
 ORIGX3
                                                               0.00000
 SCALE1 0.006516 0.000000 0.000000 SCALE2 0.000000 0.006516 0.000000 SCALE3 0.000000 0.006516
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      3.000000
      35.04
      ATOM
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      35.04
      ATOM
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      ATOM
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      73.829
      37.373
      1.00 34.42
      ATOM
      34.477
      1.00 34.75
      ATOM
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      71.925
      36.179
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      ATOM
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      37.187
      36.70
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                                                                                                       C
                                                                                                       0
                                        58.459 70.029 37.187 1.00 36.70
                                                                                                       C
                                3
 MOTA
             11 CG LYS A
                                        59.819 69.387 37.449 1.00 38.59
                                                                                                       С
                                        59.689 67.979 38.016 1.00 39.69
61.003 67.211 37.901 1.00 40.42
                                3
             12 CD LYS A
                                                                                                       C
 ATOM
             13 CE LYS A
 MOTA
                                3
                                                                                                       C
                                3
             14 NZ LYS A
                                        62.157 67.940 38.510 1.00 40.89
 MOTA
                                                                                                       N
 ATOM
             15 N
                      TYR A
                                        60.733 72.298 36.099 1.00 35.51
                                4
                                                                                                      N
             16 CA TYR A
                                        61.864 72.539 35.210 1.00 36.45
 ATOM
                                                                                                       C
                                4
 MOTA
             17 C TYR A
                                4
                                         63.081 71.752 35.695 1.00 37.94
                                                                                                       C
 MOTA
             18 0
                      TYR A
                                4
                                         63.055 71.166 36.775 1.00 38.19
                                                                                                       0
 MOTA
             19 CB TYR A
                                         62.182 74.040 35.171 1.00 34.85
                                                                                                       C
                                4
             20 CG TYR A
                                          61.071 74.870 34.566 1.00 33.25
 MOTA
                                4
                                                                                                       C
                                                      74.944 33.182 1.00 32.63
                  CD1 TYR A
 MOTA
             21
                                 4
                                          60.904
                                                                                                       C
                                                     75.545 35.375 1.00 32.51
 MOTA
                                4
                                                                                                       С
             22
                 CD2 TYR A
                                          60.158
 ATOM
                  CE1 TYR A
                                                                                                       C
             23
                                4
                                         59.850 75.670 32.618 1.00 31.87
             24 CE2 TYR A
                                                                                                      С
 MOTA
                                4
                                         59.099 76.273 34.821 1.00 32.01
 MOTA
             25 CZ TYR A
                                4
                                         58.953 76.328 33.445 1.00 31.47
                                                                                                      С
             26 OH TYR A
 MOTA
                                4
                                         57.900 77.024 32.896 1.00 31.76
                                                                                                      0
 ATOM
             27 N
                       TYR A
                                         64.144 71.733 34.898 1.00 40.06
                                5
                                                                                                      N
                                          65.351 70.998 35.272 1.00 41.80
 ATOM
             28 CA TYR A
                                5
                                                                                                       C
             29 C TYR A
                                           66.588 71.888 35.355 1.00 42.70
 ATOM
                                 5
                                                                                                       C
                                          66.654 72.941 34.719 1.00 42.98
 ATOM
             30 O
                      TYR A
                                5
                                                                                                       0
             31 CB TYR A
                                5
 ATOM
                                         65.596 69.850 34.286 1.00 42.18
                                                                                                       C
 MOTA
             32 CG TYR A
                                5
                                         64.446 68.871 34.224 1.00 42.27
                                                                                                       C
 MOTA
             33 CD1 TYR A
                                5
                                         63.238 69.225 33.630 1.00 42.61
                                                                                                       C
             34 CD2 TYR A
 MOTA
                                5
                                         64.551 67.603 34.797 1.00 42.57
                                                                                                       C
             35 CE1 TYR A
                                5
                                         62.160 68.347 33.611 1.00 42.81
 MOTA
                                                                                                      C
                                        63.478 66.715 34.783 1.00 42.46
                                5
             36 CE2 TYR A
 ATOM
                                                                                                      С
                                         62.285 67.096 34.188 1.00 42.90
             37 CZ TYR A
                                5
 ATOM
                                       61.211 66.234 34.173 1.00 42.71
             38 OH TYR A
                                5
 MOTA
```

ATOM	39	N	ASN	A	·6	67.561	71.455	36.153	1.00 43.48		N
ATOM	40	CA	ASN	A	6	68.802	72.199	36.349	1.00 44.29		С
ATOM	41	С	ASN		6	69.702	72.229	35.117	1.00 44.03		C
ATOM	42	0	ASN		6	70.291	73.263	34.800	1.00 44.49		0
ATOM	43	CB	ASN		6	69.575	71.615	37.534	1.00 45.28		C
ATOM	44	CG	ASN		6	68.911	71.909	38.867	1.00 46.42		C
ATOM	45		ASN								
					6	69.164	71.229	39.863	1.00 47.16		0
ATOM	46		ASN		6	68.065	72.935	38.895	1.00 46.63		N
MOTA	4.7	N	GLU		7	69.812	71.102	34.421	1.00 43.48		N
MOTA	48	CA	GLU		7	70.659	71.039	33.233	1.00 42.70		С
MOTA	49	C	GLU		7、	69.882	70.632	31.986	1.00 41.37		C
ATOM	50	0	GLU	A	7	68.858	69.955	32.073	1.00 40.86		0
ATOM	51	CB	GLU	A	7	71.803	70.041	33.446	1.00 44.08		С
MOTA	52	CG	GLU	Α	7	72.774	70.384	34.577	1.00 45.95		С
MOTA	53	CD	GLU	A	7	73.5 1 6	71.695	34.358	1.00 46.95		С
ATOM	54	OE1	GLU	A	7	74.048	71.911	33.246	1.00 47.35		0
MOTA	55	OE2	GLU	Α	7	73.575	72.507	35.307	1.00 48.10		0
ATOM	56	N	PRO		8	70.364	71.050	30.803	1.00 39.91		N
ATOM	57	CA	PRO		8	69.704	70.711	29.540	1.00 38.65		C
ATOM	58	C	PRO		8	70.048	69.265	29.203	1.00 37.69		C
ATOM	59	0	PRO		8	71.039					
ATOM .	60	CB	PRO				68.738	29.707	1.00 37.18		0
					8	70.324	71.698	28.559	1.00 38.70		C
ATOM	61	CG	PRO		8	71.731	71.816	29.074	1.00 39.39		C
ATOM	62	CD	PRO		8	71.529	71.926	30.570	1.00 39.63		C
ATOM	63	N	CYS		9	69.235	68.616	28.372	1.00 36.47		N
ATOM	64	CA	CYS		9	69.517	67.235	28.005	1.00 35.60		C
MOTA	65	C	CYS		9	70.554	67.179	26.882	1.00 34.44		C
ATOM	66	0	CYS	А	9	70.712	68.138	26.116	1.00 34.18		0
MOTA	67	CB	CYS	Α	9	68.226	66.497	27.617	1.00 36.20		C
MOTA	68	SG	CYS	A	9	67.191	67.270	26.369	1.00 39.57	•	S
ATOM	69	N	HIS	А	10	71.269	66.060	26.799	1.00 32.73		N
ATOM	70	CA	HIS	А	10	72.327	65.882	25.808	1.00 31.17		C
ATOM	71	С	HIS		10	72.184	64.600	24.990	1.00 30.48		C
ATOM	72	0	HIS		10	71.527	63.650	25.413	1.00 29.49		0
ATOM	73	СВ	HIS		10	73.684	65.852	26.513	1.00 31.38		C
ATOM	74	CG	HIS		10	73.953	67.049	27.368	1.00 31.58		C
ATOM	75		HIS		10	74.340	68.264	26.847	1.00 31.38	•	
ATOM	76		HIS		10						N
ATOM	77		HIS			73.893	67.217	28.710	1.00 32.22		C
					10	74.511	69.129	27.832	1.00 31.71		C
ATOM	78	NE2			10	74.245	68.518	28.972	1.00 32.26		N
ATOM	79	N	THR		11		64.580	23.822	1.00 29.90		N
MOTA	80	CA	THR		11 '	72.796	63.417	22.936	1.00 29.38	*	Ċ
MOTA	81	C	THR		11	74.134	62.681	23.054	1.00 28.79		C
ATOM	82	0	THR		11	75.057	63.175	23.699	1.00 28.16		0
ATOM	83	CB	THR		11	72.594	63.836	21.470	1.00 30.26		С
MOTA	84	OG1	THR	A	11	73.709	64.626	21.045	1.00 31.91		0
ATOM	85	CG2	THR	A	11	71.311	64.660	21.316	1.00 31.15		C
ATOM	86	N	PHE	Α	12	74.240	61.510	22.433	1.00 28.35		N
ATOM	87	CA	PHE	Α	12	75.474	60.730	22.493	1.00 28.54		С
ATOM	88	C	PHE	A	12	76.684	61.440	21.883	1.00 28.64		C
ATOM	89	0	PHE		12	77.813	61.252	22.340	1.00 27.98		0
ATOM	90	СВ	PHE		12	75.282	59.367	21.816	1.00 27.87		C
ATOM	91	CG	PHE		12	74.379	58.428	22.578	1.00 27.50		C
ATOM	92		PHE		12	74.549	58.232	23.946	1.00 27.53		C
ATOM	93		PHE		12	73.374	57.724	21.923	1.00 27.53		C
ATOM	94		PHE		12						
ATOM	95					73.729	57.348	24.652	1.00 26.85		C
111011	د د	CEZ	PHE	M	12	72.549	56.834	22.621	1.00 27.24		С

MOTA	96	CZ	PHE	A	12	72.729	56.648	23.985	1.00	26.78		С
ATOM	97	N	ASN		13	76.449	62.246	20.851		28.52		N
ATOM	98	CA	ASN		13	77.527	62.988	20.191		29.04		C
ATOM	99	C	ASN		13	78.243	63.954	21.131		28.55		C
ATOM	100	0	ASN		13	79.339	64.428	20.829		28.82		0
ATOM	101	CB	ASN		13	76.969	63.792	19.016		30.99		Ċ.
ATOM	102	CG	ASN		13	76.995	63.732	17.716		32.29		C
ATOM	103		ASN		13	76.291	63.379	16.772		34.44		0
						_						
ATOM	104		ASN		13	77.823	61.990	17.647		32.33		N
MOTA	105	N	GLU		14	77.625	64.255	22.265		27.53		N
ATOM	106	CA	GLU		14	78.218	65.190	23.212		27.62		C
ATOM	107	C	GLU		14	79.093	64.530	24.278		26.94		C
MOTA	108	0	GLU		14	79.548	65.199	25.203		27.17		0
ATOM	109	CB	GLU		14	77.114	66.003	23.890	-	28.36		C
ATOM	110	CG	GLU		14	76.224	66.769	22.912		29.57		C
MOTA	111	CD	GLU		14	75.134	67.557	23.608		30.53		С
MOTA	112				14	75.468	68.455	24.411		31.64		0
ATOM	113	OE2	GLU	A	14	73.941	67.281	23.352		31.42		0
ATOM	114	N	TYR	A	15	79.343	63.231	24.140	1.00	26.43		N
MOTA	115	CA	TYR	A	15	80.150	62.509	25.123	1.00	26.24		С
MOTA	116	C	TYR	A	15	81.325	61.721	24.555	1.00	26.03		C
ATOM	117	0	TYR	A	15	81.325	61.315	23.393	1.00	25.65		0
ATOM	118	CB	TYR	A	15	79.264	61.538	25.909	1.00	26.61		С
ATOM	119	CG	TYR	Α	15	78.257	62.197	26.818	1.00	27.62		,C
ATOM	120	CD1	TYR	A	15	78.604	62.578	28.112	1.00	28.33		C
ATOM	121		TYR		15	76.954	62.447	26.383		28.22	•	С
MOTA	122	CE1			15	77.682	63.188	28.958		29.62		C
ATOM	123		TYR		15	76.023	63.063	27.222		29.03		C
ATOM	124	CZ	TYR		15	76.395	63.429	28.505		29.97		C
ATOM	125	OH	TYR		15	75.495	64.057	29.335		31.38		0
ATOM	126	N	LEU		16	82.323	61.509	25.408		26.11		N
ATOM	127	CA	LEU		16	83.507	60.730	25.400		26.06		C
ATOM	128	C.	LEU		16	83.925	59.997	26.336		25.29		C
ATOM	129	0	LEU		16					24.34		
						83.606	60.430	27.444				0
MOTA	130	CB	LEU		16	84.660	61.628	24.607		26.91		C
ATOM	131	CG	LEU		16	84.570	62.300	23.233		28.35		C
ATOM	132		LEU		16	85.820	63.150	23.016		27.97		C
ATOM	133		LEU			84.452	61.246	22.134		28.15		C
MOTA	134	И	LEU		17	84.634	58.889	26.165		24.72		И
ATOM	135	CA	LEU		17	85.119	58.097	27.290		24.73		C
MOTA	136	C	LEU		17	86.592	58.405	27.558		24.51		C
ATOM	137	0.	LEU		17	87.386	58.553	26.626		24.84		0
ATOM	138	CB	LEU		17	84.970	56.603	26.983		24.74		С
ATOM	139	CG	LEU		17	83.551	56.029	26.964		25.01		C
ATOM	140		LEU		17	83.526	54.730	26.166		25.67		С
MOTA	141	CD2	TEU		17	83.086	55.796	28.391	1.00	25.40		C
ATOM	142	N	ILE	Α	18	86.950	58.512	28.831		24.38		N
MOTA	143	CA	ILE	А	18	88.330	58.770	29.219	1.00	24.63		С
MOTA	144	C	ILE	A	18	88.900	57.408	29.613	1.00	24.85		С
ATOM	145	0	ILE	Α	18	88.315	56.694	30.429	1.00	25.12		0
MOTA	146	CB	ILE	A	18	88.395	59.765	30.406	1.00	25.11		С
ATOM	147	CG1	ILE	Α	18	87.927	61.147	29.926	1.00	25.53		C
MOTA	148		ILE		18	89.820	59.838	30.972		24.64		С
ATOM	149		ILE		18	87.909	62.211	31.010		27.24		С
ATOM	150	N	PRO		19	90.039	57.020	29.023		25.20		N
ATOM	151	CA	PRO		19	90.652	55.723	29.332		25.63		C
MOTA	152	C	PRO		19	90.914	55.433	30.805		25.58		C
		-						22.000				-

MOTA	153	0	PRO	А	19	91.147	56.339	31.602	1.00	25.92		0
ATOM	154	CB	PRO	A	19	91.949	55.746	28.520	1.00	25.89		С
ATOM	155	CG	PRO	A	19	91.597	56.623	27.346	1.00	26.34		C
ATOM	156	CD	PRO		19	90.828	57.744	28.009	1.00	25.19		С
ATOM	157	N	GLY		20	90.847	54.150	31.149	1.00	25.25		N
ATOM	158	CA	GLY		20	91.121	53.705	32.505		25.27		C
ATOM	159	C	GLY		20	92.328	52.800	32.362		25.31		C
										24.89		0
ATOM	160	0	GLY		20	92.926	52.766	31.293				
MOTA	161	N	LEU		21	92.701	52.067	33.402		25.69		N
MOTA	162	CA	LEU		21	93.858	51.184	33.293		26.65		С
MOTA	163	C	LEU		21	93.558	49.946	32.453		26.91		C
MOTA	164	0	LEU	A	21	92.641	49.185	32.761		26.58		0
MOTA	165	CB	LEU	Α	21	94.341	50.752	34.685	1.00	26.99		С
ATOM	166	CG	LEU	Α	21	95.498	49.739	34.720	1.00	27.71		С
ATOM	167	CD1	LEU	Α	21	96.721	50.297	34.003	1.00	27.95		С
ATOM	168	CD2	LEU	A	21	95.838	49.412	36.174	1.00	28.33		С
ATOM	169	N	SER		22	94.328	49.756	31.383	1.00	27.24		N
ATOM	170	CA	SER		22	94.165	48.593	30.516		28.46		С
ATOM	171	C	SER		2.2	95.145	47.515			29.50		C
ATOM	172	0	SER		22	96.353	47.747	31.011		28.90		0
	173	CB	SER		22	94.468	48.952	29.060		28.09		C
ATOM										27.34		0
ATOM	174	OG ·	SER		22	93.577	49.931	28.573				
ATOM	175	N	THR		23	94.621	46.342	31.323		30.24		И
ATOM	176	CA	THR		23	95.448	45.231	31.790		31.35		C
ATOM	177	С	THR		23	95.902	44.337	30.642		31.61		С
ATOM	178	0	THR	A	23	95.257	44.283	29.595		32.12		0
ATOM	179	CB	THR	Α	23	94.682	44.369	32.810	1.00	31.67		C
ATOM	180	OG1	THR	Α	23	93.384	44.061	32.286	1.00	33.18		0
ATOM	181	CG2	THR	A	23	94.532	45.105	34.126	1.00	32.36		C
ATOM	182	N	VAL	A	24	97.011	43.628	30.842	1.00	32.54		N
ATOM	183	CA	VAL		24	97.537	42.746	29.805	1.00	33.28		С
ATOM	184	C	VAL		24	96.516	41.691	29.378	1.00	34.33		C
ATOM	185	0	VAL		24	96.585	41.166	28.269		34.00		0
ATOM	186	CB	VAL		24	98.837	42.025	30.267		33.25		C
ATOM	187		VAL		24	99.934	43.049	30.552		32.51		Ċ
ATOM	188		VAL		24	98.563	41.185	31.499		33.40		C
ATOM		N	ASP		25		41.392	30.253		36.01		N
	189					95.563						
ATOM	190	CA	ASP		25	94.552	40.389	29.945		38.28		C
ATOM	191	C	ASP		25	93.382	40.901	29.106		38.45		C
ATOM	192	0	ASP		25	92.550	40.114	28.668		38.94		0
ATOM	193	CB	ASP		25	94.023	39.761	31.241		40.34		C
	194`	ÇG	ASP		25	93.159	40.713	32.048		42.35		С
ATOM	195		ASP		25	91.955	40.834	31.745	1.00	44.31		0
MOTA	196	OD2	ASP		25	93.684	41.348	32.985	1.00	44.56		0
ATOM	197	N	CYS	Α	26	93.311	42.206	28.860	1.00	38.57		N
ATOM	198	CA	CYS	Α	26	92.195	42.714	28.070	1.00	38.08		С
ATOM	199	С	CYS	Α	26	92.480	42.930	26.597	1.00	38.07		C
ATOM .	200	0	CYS	Α	26	93.094	43.923	26.204	1.00	38.02		0
ATOM	201	CB	CYS		26	91.652	44.026	28.639		37.39		С
ATOM	202	SG	CYS		26	89.947	44.430	28.092		36.98		s
ATOM	203	N	ILE		27	92.025	41.982	25.789		37.71		N
ATOM	204	CA	ILE		27	92.144	42.070	24.347		37.96	`	C
ATOM	205	CA	ILE		27	90.721	41.819	23.871		37.64		C
,								24.526		37.26		0
ATOM	206	O	ILE		27	89.965	41.100					
ATOM	207	CB	ILE		27	93.099	40.999	23.765		38.64		C
ATOM	208		ILE		27	92.780	39.627	24.361		38.53		C
ATOM	209	CG2	ILE	A	27	94.548	41.407	24.020	1.00	38.05		C

7 mov	010	an.	TT 13	70	22	02 (20	20 504	23.789	1 00	39.94		C
MOTA	210		ILE		27	93.629	38.504					
ATOM	211	N	PRO		28	90.329	42.424	22.742		37.48		N
MOTA	212	CA	PRO	A	28	88.985	42.267	22.185		37.27		С
MOTA	213	C	PRO	Α	28	88.399	40.862	22.281	1.00	37.00		С
ATOM	214	0	PRO	Α	28	87.245	40.696	22.675	1.00	36.24		0
MOTA	215	CB	PRO	Α	28	89.165	42.726	20.741	1.00	37.74		C
ATOM	216	CG	PRO		28	90.147	43.838	20.892	1.00	37.23		С
ATOM	217	CD	PRO		28	91.165	43.259	21.858		37.69		C
					29	89.195	39.854	21.934		36.71		N
ATOM	218	N	SER					21.960		36.44		C
MOTA	219	CA	SER		29	88.724	38.473					C
MOTA	220	C	SER		29	88.358	37.934	23.340		35.69		
MOTA	221	0	SER		29	87.608	36.964	23.444		35.87		0
ATOM	222	CB	SER	A	29	89.747	37.543	21.291		37.16		C
MOTA	223	OG	SER	Α	29	91.019	37.620	21.907	1.00	38.53		0
ATOM	224	N	ASN	Α	30	88.874	38.547	24.400	1.00	34.53		N
ATOM	225	CA	ASN	Α	30	88.541	38.084	25.744	1.00	33.29		С
ATOM	226	С	ASN	Α	30	87.358	38.850	26.342	1.00	31.44		C
ATOM	227	0	ASN		30	86.903	38.526	27.436	1.00	31.19		0
ATOM	228	CB	ASN		30	89.747	38.195	26.686		35.35		C
ATOM	229	CG	ASN		30	90.819	37.158	26.396		37.30		С
			ASN		30	90.517	36.011	26.061		38.46		Ö
ATOM	230											N
ATOM	231		ASN		30	92.078	37.552	26.544		37.96		
ATOM	232	N	VAL		31	86.861	39.858	25.628		28.79		N
MOTA	233	CA	VAL		31	85.730	40.645	26.119		27.05		C
MOTA	234	С	VAL	А	31	84.408	39.897	25.955		26.82		C
ATOM	235	0	VAL	Α	31	84.095	39.394	24.880		26.06		0
ATOM	236	CB	VAL	A	31	85.637	42.011	25.400		26.53		С
ATOM	237	CG1	VAL	Α	31	84.345	42.724	25.797	1.00	25.95		С
ATOM	238	CG2	VAL	Α	31	86.845	42.873	25.773	1.00	24.71		C
ATOM	239	N	ASN	А	32	83.645	39.835	27.041	1.00	26.34	•	N
ATOM	240	CA	ASN		32	82.355	39.140	27.082	1.00	26.00		C
ATOM	241	C	ASN		32	81.227	40.164	26.965		25.15		С
ATOM	242	Ō	ASN		32	81.080	41.016	27.842		25.29		0
		CB	ASN		32	82.240	38.396	28.420		26.75		C
ATOM	243					80.958	37.583	28.549		28.49		C
ATOM	244	CG.	ASN		32			27.884		28.21		0
ATOM	245		ASN		32	79.957	37.851					
MOTA	246		ASN		32	80.984	36.591	29.434	1.00			N
MOTA	247	N	LEU		33	80.429	40.079			24.40	1	N
	248	CÀ	LEU		33	79.329	41.024	25.700		24.28		C
MOTA	249	С	LEU	Α	33	77.947	40.492	26.094		23.96		C
MOTA	250	0	LEU	Α	33	76.922	41.024	25.664	1.00	23.48		0
MOTA	251	CB	LEU	A	33	79.300	41.511	24.242		24.79		C
ATOM	252	CG	LEU	Α	33	80.520	42.316	23.774	1.00	25.38		С
MOTA	253	CD1	LEU	Α	33	80.321	42.761	22.333	1.00	25.52		C
ATOM	254		LEU		33	80.721	43.529	24.675	1.00	25.70		С
ATOM	255	N	SER		34	77.920	39.445	26.913	1.00	23.29		N
ATOM	256	CA	SER		34	76.653	38.882	27.375		23.29		C
ATOM	257	C	SER		34	75.916	39.961	28.168		22.23		C
ATOM	258	0	SER		34	76.544	40.817	28.780		22.07		0
							37.670			23.70		C
MOTA	259	CB	SER		34	76.909		28.278				0
MOTA	260	OG	SER		34	75.698	37.216	28.861		27.20		
MOTA	261	N	THR		35	74.588	39.923	28.170		21.87		N
MOTA	262	CA	THR		35	73.822	40.925	28.902		20.75		C
ATOM	263	C	THR		35	72.396	40.419	29.149		20.94		C
MOTA	264	0	THR	A	35	71.826	39.699	28.320		21.27		0
MOTA	265	CB	THR	A	35	73.814	42.277	28.112		21.38		. C
ATOM	266	OG1	THR	A	35	73.523	43.368	29.001	1.00	21.23		0

ATOM	267	CG2	THR	Δ	35	72.786	42.239	26.991	1.00	20.66			С
ATOM	268	N	PRO		36	71.801	40.786	30.296		20.32			N
	269	CA	PRO		36	70.440	40.354	30.636		20.69			C
ATOM													
ATOM	270	C	PRO		36	69.338	41.049	29.841		20.70			C
ATOM	271	0	PRO		36	69.404	42.251	29.581		21.51			0
ATOM	272	CB	PRO		36	70.350	40.662	32.128		19.89			С
ATOM	273	CG	PRO	A	36	71.153	41.919	32.239		19.69			C
MOTA	274	CD	PRO	Α	36	72.372	41.614	31.377	1.00	20.06			C
ATOM	275	N	LEU	A	37	68.317	40.285	29.471	1.00	21.00			N
ATOM	276	CA	LEU	Α	37	67.197	40.830	28.718	1.00	21.84			C
ATOM	277	C	LEU	Α	37	65.980	41.072	29.609	1.00	21.93			С
ATOM	278	0	LEU	Α	37	65.257	42.049	29.416	1.00	21.26			0
ATOM	279	CB	LEU		37	66.798	39.882	27.582	1.00	22.24			С
ATOM	280	CG	LEU		37	65.696	40.404	26.650		22.01			С
ATOM	281		LEU		37	66.269	41.525	25.787		22.09			C
ATOM	282		LEU		37	65.164	39.289	25.777		22.26			C
										21.79			N
ATOM	283	N	VAL.		38	65.758	40.193	30.585					C
ATOM	284	CA	VAL		38	64.598	40.328	31.466		22.14			
ATOM	285	C	VAL		38	64.950	40.384	32.950		22.71			C
ATOM	286	0	VAL		38	65.973	39.846	33.386		22.81			0
ATOM	287	CB	VAL		38.	63.577	39.188	31.216		22.25			С
ATOM	288	CG1	VAL	Α	38	63.064	39.267	29.776	1.00	22.95			C
ATOM	289	CG2	VAL	Α	38	64.220	37.832	31.469	1.00	22.56		•	C
ATOM	290	N	LYS	A	39	64.081	41.032	33.719	1.00	22.22			N
ATOM	291	CA	LYS	A	39	64.296	41.230	35.144	1.00	22.61			С
ATOM	292	C	LYS		39	64.525	39.970	35.972	1.00	22.81			С
ATOM	293	0	LYS		39	64.018	38.892	35.655		22.94			0
ATOM	294	CB	LYS		39	63.130	42.019	35.750		22.84			С
ATOM	295	CG	LYS		39	61.814	41.259	35.802		23.34			C
ATOM	296	CD	LYS		39	60.751	42.061	36.548		25.09			C
					39	59.425	41.313	36.606		25.38			C
ATOM	297	CE	LYS							26.79			N
ATOM	298	NZ	LYS		39	58.393	42.105	37.328					
ATOM	299	N	PHE		40	65.297	40.140	37.041		23.12			N
ATOM	300	CA	PHE		40	65.620	39.065	37.973		24.28			C
MOTA	301	C	PHE		40	65.900	39.689	39.342		25.44			C
ATOM	302 ~	0	PHE		40	66.044	40.914	39.456		26.48			0
ATOM	303	CB	PHE	Α	40	66.848	38.272	37.492		22.73			С
MOTA	304	CG	PHE	А	40	68.061	39.123	37.217		22.77			С
MOTA	305	CD1	PHE	А	40	68.251	39.709	35.965	1.00	22.17			С
ATOM	306	CD2	PHE	A	40	69.011	39.347	38.212		22.45			С
MOTA	307	CE1	PHE	A	40	69.369	40.504	35.709	1.00	22.24			C
ATOM	308	CE2	PHE	Α	40	70.133	40.139	37.971	1.00	22.30			С
ATOM	309	CZ	PHE	A	40	70.313	40.721	36.713	1.00	23.25			C
MOTA	310	N	GLN		41	65.968	38.850	40.373	1.00	25.99			N
ATOM	311	CA	GLN		41	66.233	39.300	41.741	1.00	27.32			C
MOTA	312	C	GLN		41	67.722	39.323	42.021		26.58			С
ATOM	313	Ō	GLN		41	68.494	38.644	41.350		26.05			0
ATOM	314	CB	GLN		41	65.580	38.360	42.767		28.63			C
ATOM	315	CG	GLN		41	64073	38.418	42.811		32.62			C
ATOM	316	CD	GLN		41	63.568	39.766	43.273		34.57			C
								44.429			•		0
ATOM	317		GLN		41	63.767	40.164			37.98			
ATOM	318		GLN		41	62.915	40.485	42.375		35.13			N
ATOM	319	N	LYS		42	68.112	40.091	43.035		26.17			N
MOTA	320	CA	LYS		42	69.511	40.189	43.432		26.88			C
MOTA	321	C	LYS		42	70.104	38.790	43.624		26.18			C
ATOM	322	0	LYS		42	69.506	37.936	44.284		25.24			0
ATOM	323	CB	LYS	A	42	69.620	40.984	44.738	1.00	28.70			С

MOTA	324	CG	LYS	Α	42	71.020	41.076	45.320	1.00 30.39	С
MOTA	325	CD	LYS	Α	42	71.018	41.936	46.581	1.00 32.90	C
MOTA	326	CE	LYS	Α	42	72.414	42.059	47.174	1.00 34.17	C
ATOM	327	NZ	LYS	Α	42	72.429	42.982	48.349	1.00 36.34	N
ATOM	328	N	GLY	Α	43	71.271	38.561	43.031	1.00 25.61	N
ATOM	329	CA	GLY	Α	43	71.929	37.272	43.157	1.00 25.50	C
ATOM	330	С	GLY	Α	43	71.574	36.267	42.079	1.00 24.98	C
MOTA	331	0	GLY	Α	43	72.260	35.260	41.916	1.00 25.00	0
ATOM	332	N	GLN		44	70.500	36.523	41.343	1.00 24.55	N
MOTA	333	CA	GLN	Α	44	70.092	35.606	40.287	1.00.24.65	C
ATOM	334	С	GLN		44	70.707	36, 017	38.961	1.00 25.02	C
ATOM	335	0	GLN		44	71.394	37.029	38.868	1.00 24.74	0
ATOM	336	СВ	GLN		44	68.569	35.610	40.117	1.00 24.74	C
ATOM	337	CG	GLN		44	67.766	35.374	41.390	1.00 24.75	C
ATOM	338	CD	GLN		44	66.270	35.328	41.124	1.00 24.40	
ATOM	339		GLN		44	65.758	36.043	40.255	1.00 23.33	C
ATOM	340	NE2			44	65.557	34.499	41.884	1.00 24.07	0
ATOM	341	N	GLN		45	70.452	35.208		1.00 24.73	N
ATOM	342	CA	GLN		45	70.432		37.942		N
ATOM	343	C	GLN		45	~69.584	35.490	36.584	1.00 26.47	C
ATOM	. 344	0	GLN		45	-	35.679	35.834	1.00 25.54	C
ATOM	345	СВ	GLN			68.559	35.137	36.242	1.00 24.56	 0
ATOM	345	CG	GLN		45	71.650	34.298	35.982	1.00 28.94	C
ATOM	347	CD			45	73.051	34.092	36.532	1.00 31.95	C
ATOM		OE1	GLN		45	73.946	35.287	36.280	1.00 34.21	С
	348				45	74.117	35.716	35.137	1.00 36.26	0
ATOM	349		GLN		45	74.525	35.834	37.348	1.00 35.09	N
ATOM	350	N	SER		46	69.597	36.458	34.759	1.00 24.88	N
MOTA	351	CA	SER		46	68.379	36.643	33.986	1.00 24.59	C
ATOM	352	C	SER		46	68.038	35.329	33.287	1.00 25.11	C
ATOM	353	. 0	SER		46	68.937	34.576	32.907	1.00 24.15	0
ATOM	354	CB	SER		46	68.567	37.732	32.931	1.00 23.51	C
ATOM	355	OG	SER		46	67.375	37.895	32.188	1.00 22.66	0
ATOM	356	N	GLU		47	66.747	35.052	33.122	1.00 26.17	N
ATOM	357	CA	GLU		47	66.318	33.831	32.443	1.00 27.54	C
MOTA	358	C .	GLU		47	66.708	33.896	30.970	1.00 27.30	C
MOTA	359	0	GLU		47	66.831	32.871	30.303	1.00 27.84	0
MOTA	360	CB	GLU		47	64.803	33.649	32.564	1.00 29.20	C
MOTA	361	CG	GLU		47	64.330	33.359	33.977	1.00 32.39	C
MOTA	362	CD	GLŲ		47	62.821	33.411	34.104	1.00 34.34	С
MOTA	363		GLU		.47	62.145	32.508	33.566	1.00 35.91	0
MOTA	364	OE2	GLU		47	62.314	34.363	34.735	1.00 35.54	0
MOTA	365	N	ILE		48	66.890	35.109	30.458	1.00 26.04	N
MOTA	366	CA	ILE	A	48	67.284	35.284	29.063	1.00 25.89	C
MOTA	367	C	ILE	А	48	68.454	36.254	28.971	1.00 25.55	C
ATOM	368	0	ILE	Α	48	68.353	37.409	29.387	1.00 25.22	0
MOTA	369	CB	ILE	Α	48	66.133	35.844	28.193	1.00 26.14	С
ATOM	370	CG1	ILE	Α	48	64.913	34.921	28.255	1.00 27.04	С
MOTA	371	CG2	ILE	Α	48	66.604	35.977	26.747	1.00 25.69	С
MOTA	372	CD1	ILE	Α	48	63.686	35.502	27.561 ⁻	1.00 28.89	С
ATOM	373	N	ASN	Α	49	69.567	35.775	28.431	1.00 24.84	N
MOTA	374	CA	ASN	Α	49	70.750	36.603	28.277	1.00 24.41	C
MOTA	375	C	ASN	Α	49	71.148	36.668	26.813	1.00 24.16	C
MOTA	376	0	ASN	A	49	71.297	35.637	26.157	1.00 24.28	0
ATOM	377	CB	ASN		49	71.914	36.030	29.095	1.00 24.39	C
MOTA	378	CG	ASN		49	71.693	36.157	30.592	1.00 25.36	c
MOTA	379	OD1	ASN		49	71.883	37.227	31.175	1.00 23.83	0
ATOM	380		ASN		49	71.273	35.065	31.219	1.00 25.54	N
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MOTA	381	N	LEU	Α	50	71.298	37.879	26.292	1.00 23.32			N
MOTA	382	CA	LEU	A	50	71.724	38:045	24.909	1.00 23.00			С
ATOM	383	C	LEU	A	50	73.222	37.769	24.916	1.00 23.10			С
ATOM	384	0	LEU	A	50	73.873	37.953	25.945	1.00 22.63			0
ATOM	385	CB	LEU	A	50	71.492	39.484	24.442	1.00 22.34			С
ATOM	386	CG	LEU		50	70.087	40.075	24.569	1.00 22.93			C
ATOM	387	CD1			50	70.100	41.515	24.045	1.00 23.23			Ċ
ATOM	388	CD2	LEU		50	69.093	39.221	23.787	1.00 23.68			C
ATOM	389	N	LYS			.73.769	37.322	23.788	1.00 23.53			N
ATOM	390	CA	LYS		51	75.201	37.074	23.707	1.00 24.58			C
ATOM	391	C	LYS		51	75.900	38.353	23.240	1.00 24.53			C
ATOM	392	0	LYS		51	77.099	38.525	23.448	1.00 24.51			0
ATOM	393	CB	LYS		51	75.492	35.878	22.789	1.00 24.31	•		C
ATOM	394	CG	LYS		51	75.057	34.561	23.438	1.00 20.20			C
ATOM	395	CD	LYS		51	75.469	33.337	22.639	1.00 27.03			C
ATOM	396	CE	LYS		51			23.324	1.00 29.52			C
ATOM	397	NZ				74.978	32.065				•	
ATOM	398	N N	LYS		51 52	75.354	30.839 39.240	22.555 22.596	1.00 32.78			N
						75.139			1.00 23.97			N
ATOM	399	CA	ILE		52	75.641	40.555	22.192	1.00 23.86			C
ATOM	400	C	ILE		52	74.496	41.505	22.570	1.00 23.49			C
ATOM	401	0	ILE		52	73.322	41.143	22.469	1.00 24.41			0
ATOM	402	CB	ILE		52	75.985	40.667	20.678	1.00 24.09			C
ATOM	403	CG1	ILE		52	74.760	40.365	19.815	1.00 24.55			C
MOTA	404	CG2	ILE		52	77.174	39.749	20.352	1.00 24.63			С
ATOM	405		ILE		52	74.985	40.668	18.337	1.00 25.99			С
ATOM	406	N	PRO		53	74.821	42.722	23.019	1.00 22.93			N
ATOM	407	CA	PRO		53	73.827	43.720	23.437	1.00 22.98			С
ATOM	408	C	PRO		53	73.051	44.482	22.363	1.00 23.03			С
MOTA	409	0	PRO		53	72.673	45.631	22.586	1.00 23.64			0
ATOM	410	CB	PRO		53	74.654	44.657	24.305	1.00 22.57			C
MOTA	411	CG	PRO	Α	53	75.944	44.714	23.542	1.00 23.54			G.
ATOM	412	CD	PRO	А	53	76.190	43.246	23.194	1.00 23.09			С
MOTA	413	N	LEU	Α	54	72.798	43.853	21.220	1.00 22.71			N
ATOM	414	CA	LEU	Α	54	72.073	44.521	20.138	1.00 23.22	•		С
MOTA	415	C	LEU	Α	54	70.760	43.834	19.777	1.00 22.95			С
MOTA	416	0	LEU	Α	54	70.715	42.615	19.596	1.00 22.05	*		0
MOTA	417	CB	LEU	Α	54	72.940	44.589	18.870	1.00 23.59			С
ATOM	418	CG	LEU	Α	54	74.366	45.141	18.963	1.00 23.98			С
ATOM	419	CD1	LEU	A	54	75.015	45.095	17.583	1.00 24.50			C
ATOM	420	CD2	LEU	A:	54	74.343	46.567	19.494	1.00 24.21			С
ATOM	421	N	VAL	Α	55	69.695	44.625	19.675	1.00 22.53			N
ATOM	422	CA	VAL	Α	55	68.392	44.104	19.284	1.00 22.49			С
ATOM	423	C	VAL	A	55	67.871	45.017	18.170	1.00 22.61			С
ATOM	424	0	VAL	A	55	68.116	46.229	18.183	1.00 22.47			0
ATOM	425	CB	VAL		55	67.387	44.060	20.475	1.00 22.79			С
ATOM	426	CG1	VAL		55	68.032	43.361	21.673	1.00 22.48			С
ATOM	427		VAL		55	66.924	45.452	20.845	1.00 22.85			C
ATOM	428	N	SER		56	67.180	44.438	17.193	1.00 22.42			N
ATOM	429	CA	SER		56	66.665	45.232	16.080	1.00 22.42			C
ATOM	430	C	SER		56	65.300	45.823	16.410	1.00 22.63	•		C
ATOM	431	0	SER		56	64.485	45.200	17.094	1.00 23.01			0
ATOM	432	CB	SER		56	66.611	44.389	14.794	1.00 22.36			C
ATOM	433	OG	SER		56	65.832	43.220	14.754	1.00 22.30			0
ATOM	434	И	ALA		57	65.076	47.039	15.921	1.00 23.60			N
ATOM	435	CA	ALA		57	63.853	47.039	16.163	1.00 22.02			C
ATOM	436	C	ALA		57	62.557	47.133	15.730	1.00 22.37			C
ATOM	437	0	ALA		57	62.537	46.338					0
111011	± J /	J	TTY.	7	<i>.</i> .	92.933	40.330	14.781	1.00 24.23			J

ATOM	438		ALA		57	63.971	49.174	15.496	1.00 21.89		C
MOTA	439	N	ILE		58	61.480	47.430	16.444	1.00 24.06		N C
MOTA	440	CA	ILE		58	60.161	46.860	16.174	1.00 24.95		C
MOTA	441	C	ILE		58	59.552	47.647	15.016	1.00 25.14		0
MOTA	442	0	ILE		58	58.567	48.369	15.189	1.00 25.13		
MOTA	443	CB	ILE	Α	58	59.259	46.984	17.427	1.00 25.04		С
ATOM	444	CG1	ILE	A	58	60.035	46.504	18.661	1.00 25.04		C
MOTA	445	CG2	ILE		58	57.992	46.149	17.260	1.00 25.28		C
ATOM	446	CD1.	ILE	Α	58	59.239	46.529	19.950	1.00 24.84		C
ATOM	447	N	MET	Α	59	60.143	47.483	13.834	1.00 25.33		N
MOTA	448	CA	MET	Α	59	59.716	48.220	12.647	1.00 25.63		C
ATOM	449	С	MET	Α	59	59.521	47.358	11.398	1.00 25.77		C
ATOM	450	0	MET	Α	59	60.257	46.397	11.171	1.00 25.17		0
ATOM	451	CB	MET	Α	59	60.750	49.310	12.354	1.00 25.44		C
MOTA	452	CG	MET	Α	59	61.021	50.234	13.540	1.00 24.70		C
ATOM	453	SD	MET	Α	59	62.394	51.382	13.288	1.00 24.28		s
MOTA	454	CE	MET	Α	59	61.721	52.448	11.981	1.00 24.30		С
MOTA	455	N	GLN	Α	60	58.533	47.724	10.585	1.00 26.54		N
MOTA	456	CA	GLN	Α	6.0	58.234	47.005	9.345	1.00 27.32		C
MOTA	457	C	GLN	Α	60	59.464	46.961	8.443	1.00 27.38		С
ATOM	458	0	GLN	Α	60	59.719	45.963	7.771	1.00 27.43		0
MOTA	459	CB	GLN	Α	60	57.109	47.701	8.564	1.00 27.95		С
MOTA	460	CG	GLN	Α	60	55.838	47.994	9.337	1.00 29.68		C
MOTA	461	CD	GLN	Α	60	54.802	48.717	8.482	1.00 31.25		С
ATOM	462	OE1	GLN	Α	60	55.149	49.525	7.616	1.00 31.26		0
ATOM	463	NE2	GLN	Α	60	53.526	48.442	8.735	1.00 31.01		N
ATOM	464	N	SER	Α	61	60.220	48.053	8.427	1.00 27.19		N
ATOM	465	CA	SER	Α	61	61.398	48.145	7.573	1.00 27.60		С
MOTA	466	C	SER	Α	61	62.682	47.598	8.193	1.00 27.60		С
ATOM	467	0	SER	Α	61	63.773	47.818	7.662	1.00 28.23		0
MOTA	468	CB	SER	Α	61	61.620	49.602	7.152	1.00 27.83		С
ATOM	469	OG	SER	Α	61	61.955	50.422	8.261	1.00 29.04		0
ATOM	470	N	VAL	Α	62	62.560	46.867	9.296	1.00 26.86		N
MOTA	471	CA	VAL	Α	62	63.745	46.337	9.957	1.00 26.42		С
MOTA	472	C	VAL	Α	62	63.665	44.883	10.402	1.00 26.63		C
MOTA	473	0	VAL	Α	62	64.432	44.045	9.938	1.00 27.23		0
MOTA	474	CB	VAL	A	62	64.098	47.181	11.210	1.00 26.30		C
MOTA	475	CG1	VAL	Α	-62	65.342	46.618	11.893	1.00 25.75		С
ATOM	476	CG2	VAL	A	62	64.310	48.631	10.820	1.00 25.78	、.	С
MOTA	477	N	SER	Α	63	62.725	44.585	11.291	1.00 26.87	(И
ATOM	478	CA	SER	Α	63	62.621	43.248	11.849	1.00 26.97		C
ATOM	479	С	SER	Α	63	61.630	42.252	11.253	1.00 27.37		С
ATOM	480	0	SER	Α	63	60.534	42.048	11.778	1.00 26.24		0
MOTA	481	CB	SER	Α	63	62.394	43.364	.13.359	1.00 27.27		C
ATOM	482	OG	SER	A	63	63.447	44.106	13.965	1.00 27.97		0
ATOM	483	N	GLY	A	64	62.049	41.627	10.158	1.00 27.73		N
MOTA	484	CA	GLY	Α	64	61.248	40.610	9.507	1.00 28.60		С
ATOM	485	С	GLY		64	61.899	39.284	9.859	1.00 29.32		С
MOTA	486	0	GLY	Α	64	62.870	39.257	10.623	1.00 28.30		. 0
ATOM	487	N	GLU		65	61.387	38.190	9.304	1.00 29.97		N
ATOM	488	CA	GLU		65	61.912	36.855	9.584	1.00 31.24		C
ATOM	489	С	GLU		65	63.413	36.688	9.339	1.00 30.93		С
MOTA	490	0	GLU		65	64.131	36.167	10.188	1.00 30.06		0
ATOM	491	СВ	GLU		65	61.147	35.811	8.760	1.00 33.66		C
ATOM	492	CG	GLU		65	60.983	36.196	7.292	1.00 37.41		C
ATOM	493	CD	GLU		65	59.788	37.106	7.051	1.00 39.43		C
ATOM	494		GLU		65	58.650	36.587	7.069	1.00 41.83		0
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MOTA	495	OE2	GLU	A	65	59.978	38.331	6.846	1.00 40.38		0
MOTA	496	N	LYS		66	63.884	37.123	8.176	1.00 30.29		N
ATOM	497	CA	LYS		66	65.295	36.996	7.837	1.00 30.29		C
ATOM	498	С	LYS		66	66.221	37.768	8.781	1.00 29.26		С
MOTA	499	0	LYS		66	67.294	37.284	9.140	1.00 28.41		0
ATOM	500	CB	LYS		66	65.528	37.423	6.380	1.00 31.58	-	С
ATOM	501	CG	LYS		66	64.731	38.637	5.917	1.00 33.89		C
ATOM	502	CD	LYS		66	63.214	38.395	5.941	1.00 34.74		С
ATOM	503	CE	LYS		66	62.489	39.441	5.136	1.00 35.36	•	С
ATOM	504	NZ	LYS		66	62.985	39.417	3.718	1.00 34.63		N
ATOM	505	N	MET		67	65.807	38.962	9.185	1.00 28.14		N
ATOM	506	CA	MET		67 67	66.606	39.765	10.104	1.00 26.95		C
ATOM ATOM	507 508	C	MET		67	66.722	39.019	11.433	1.00 26.58		C
ATOM	509	O CB	MET MET		67 67	67.812	38.889	11.997	1.00 25.12		0
ATOM	510	CG	MET		67	65.939 66.628	41.125 42.020	10.327 11.347	1.00 27.01		C
ATOM	511	SD	MET		67	68.293	42.020		1.00 25.99		C
ATOM	512	CE	MET		67	67.950	42.472	10.859 9.432	1.00 26.26 1.00 25.77		S C
ATOM	513	N	ALA		68	65.587	38.513	11.910	1.00 25.77		N
ATOM	514	CA	ALA		68 ·	65.524	37.791	13.174	1.00 26.72	•	C
ATOM	515	C	ALA		68	66.457	36.590	13.174	1.00 23.82		C
ATOM	516	o	ALA		68	67.092	36.315	14.217	1.00 27.20		0
ATOM	517	CB	ALA		68	64.092	37.350	13.452	1.00 27.21		C
ATOM	518	N	ILE		69	66.532	35.867	12.092	1.00 27.20		N
ATOM	519	CA	ILE		69	67.403	34.702	12.011	1.00 27.15		C
ATOM	520	С	ILE		69	68.870	35.125	11.980	1.00 26.50		c
MOTA		. 0	ILE		69	69.700	34.568	12.695	1.00 27.23		0
ATOM	522	CB	ILE		69	67.089	33.867	10.747	1.00 27.71		C
ATOM	523	CG1	ILE	A	69	65.692	33.250	10.870	1.00 28.00		C
ATOM	524	CG2	ILE		69	68.144	32.787	10.558	1.00 27.79		C
MOTA	525	CD1	ILE	A	69	65.121	32.737	9.547	1.00 29.43		C
ATOM	526	N	ALA	Α	70	69.184	36.116	11.154	1.00 25.73		N
MOTA	527	CA.	ALA	Α	70	70.556	36.592	11.029	1.00 25.41		С
ATOM	528	C	ALA	Α	70	71.109	37.181	12.325	1.00 25.00		С
MOTA	529	0	ALA	А	70	72.260	36.936	12.683	1.00 24.51		0
ATOM	530	CB	ALA	А	70	70.645	37.627	9.914	1.00 25.47		С
MOTA	531	N	LEU	Α	71	70.292	37.961	13.025	1.00 24.62		N
ATOM	532	CA	LEU		71.	70.736	38.580	14.266	1.00 24.36		C
MOTA	533	C	LEU		. 71	70.878	37.541	15.372	1.00 24.81		С
ATOM	534	0	LEU		71	71.850	37.562	16.121	1.00 25.09		0
ATOM	535	CB	LEU		71	69.759	39.680	14.690	1.00 23.62		C.
ATOM	536	CG	LEU		71	70.116	40.466	15.960	1.00 23.09		C
ATOM	537		LEU		71	71.583	40.872	15.932	1.00 22.51		С
ATOM	538		LEU		71	69.220	41.701	16.053	1.00 22.83		С
ATOM	539	N	ALA		72	69.916	36.629	15.471	1.00 25.59		N
ATOM	540	CA	ALA		72	69.982	35.583	16.490	1.00 26.49		C
ATOM	541	С	ALA		72	71.246	34.742	16.284	1.00 27.18		C
MOTA MOTA	542 543	O	ALA		72 72	71.868	34.287	17.249	1.00 26.99		0
ATOM	544	CB N	ALA ARG		72 73	68.739	34.699	16.421	1.00 26.25		C
ATOM	545	CA	ARG		73 73	71.624 72.822	34.540	15.025 14.707	1.00 27.93		N
ATOM	546	CA	ARG		73 73	74.084	33.765 34.417	15.267	1.00 28.79 1.00 28.77		C C
ATOM	547	0	ARG		73 73	75.058	34.417	15.267	1.00 28.77		0
ATOM	548	CB	ARG		73 73	72.965	33.729	13.191	1.00 28.68		C
ATOM	549	CG	ARG		73 73	72.963	32.535	12.601	1.00 30.52		C
ATOM	550	CD.	ARG		73	72.198	32.469	11.089	1.00 33.48		C
ATOM	551	NE	ARG		73	71.517	31.303	10.534	1.00 35.40		N
							32.303	10.004	2.00 55.10		7.4

ATOM	552	CZ	ARG	2	73	71.257	31.135	9.241	1 00	26 92		С
ATOM	553		ARG		73	71.618	32.061	8.360		37.07		N
ATOM	554		ARG		73	70.642	30.034	8.825		37.30	,	N
ATOM	555	N	GLU		74	74.064	35.741	15.401		28.39	-	N
ATOM	556	CA	GLU	Α	74	75.210	36.470	15.933	1.00	28.09		C
ATOM	557 ·	C	GLU	Α	74	75.100	36.720	17.444	1.00	27.22		C
ATOM	558	0	GLU	Α	74	75.977	37.342	18.034	1.00	27.15		0
ATOM	559	CB	GLU		74	75.378	37.804	15.195		30.01		C
ATOM	560	CG	GLU		74	75.546	37.668	13.679		32.33		C
ATOM	561	CD	GLU		74	76.686						
							36.741	13.283		33.71		C
ATOM	562		GLU		74	77.836	36.984	13.704		36.00		0
ATOM	563		GLU		74	76.431	35.768	12.543		35.10		0
ATOM	564	N	GLY	Α	75	74.021	36.251	18.066	1.00	26.36		N
ATOM	565	CA	GLY	Α	75	73.872	36.427	19.504	1.00	25.20		C
MOTA	566	C	GLY	Α	75	72.872	37.461	19.993	1.00	24.86		С
ATOM	567	0	GLY	Α	75	72.677	37.607	21.200	1.00	24.26		0
ATOM	568	N	GLY			72.238	38.179	19.070		24.23		N
	569	CA	GLY		76	71.266	39.186	19.464		24.11		C
ATOM	570	C	GLY		76							C
						69.848	38.706	19.237		23.43		
ATOM	571		GLY		76	69.627	37.531	18.963		23.27	•	0
MOTA	572	N	ILE		77	68.876	39.604	19.346		23.31	•	N
ATOM	573	CA	ILE	Α	77	67.494	39.205	19.127		22.63		C
ATOM	574	C	ILE	Α	77	66.718	40.293	18.391	1.00	23.12		С
ATOM	575	0	ILE	A	77	66.984	41.487	18.563	1.00	22.23		0
ATOM	576	CB	ILE	A	77	66.797	38.873	20.470	1.00	22.89		С
ATOM	577	CG1	ILE	A	77	65.535	38.044	20.212	1.00	22.47		C
ATOM	578	CG2	ILE		77	66.465	40.163	21.230		22.43		C
ATOM	579		ILE		77	64.847	37.547	21.474		21.82		C
ATOM	580		SER									
		N			78	65.771	39.873	17.556		23.10		N
ATOM	581	CA	SER		78	64.942	40.813	16.809		23.37		С
ATOM	582	С	SER		78	63.526	40.796	17.362		23.52		С
MOTA	583	0	SER	A	78	63.044	39.762	17.820	1.00	24.10		0
ATOM	584	CB	SER	A	78	64.877	40.434	15.321	1.00	23.20		C
MOTA	585	OG	SER	Α	78	66.125	40.583	14.671	1.00	24.07		0
MOTA	586	N	PHE	Α	79	62.863	41.944	17.328	1.00	23.99		N
ATOM	587	CA	PHE	Α	79	61.483	42.020	17.777	1.00	24.76		С
ATOM	588	С	PHE	Α	79	60.617	42.208	16.534		24.96		С
MOTA	589	0	PHE		79	60.474	43.321	16.031		24.87		Ö
ATOM	590	CB	PHE		79	61.284	43.183	18.760		24.45		C
ATOM	591	CG	PHE		79	61.820	42.905	20.137				
										-24.94	٠.	. C
ATOM	592		PHE		79	63.161	43.126	20.438		25.40		C
ATOM	593		PHE		79	60.993	42.367	21.121		25.21		С
ATOM	594		PHE		79	63.674	42.812	21.699	1.00	25.47		C
ATOM	595		PHE	Α	79	61.496	42.050	22.382	1.00	25.32		C
MOTA	596	CZ	PHE	Α	79	62.839	42.272	22.670	1.00	24.97		C
ATOM	597	N	ILE	Α	80	60.060	41.108	16.033	1.00	25.49		N
ATOM	598	CA	ILE		80	59.212	41.134	14.837		25.86		С
MOTA	599	C	ILE		80	58.160	42.236	14.964		25.66		C
ATOM	600	Ō	ILE		80	57.435	42.294	15.961		24.99		Ö
ATOM	601	CB	ILE		80	58.496	39.775	14.634		26.44		C
ATOM	602		ILE		80	59.527	38.640	14.575		26.91		C
ATOM	603		ILE		80	57.658	39.810	13.353		26.85		C
MOTA	604	CD1	ILE	A	80	60.497	38.729	13.410	1.00	27.62		C
ATOM	605	N	PHE	Α	81	58.064	43.101	13.955	1.00	25.74		N
ATOM	606	CA	PHE	Α	81	57.107	44.202	14.020		26.34		C
ATOM	607	С	PHE		81	55.665	43.759	14.221		26.79		C
ATOM	608	0	PHE		81	55.234	42.737	13.688		26.54		O
	•	-			_		,_,		1.00	20.74		9

ATOM	609	CB	PHE		81	57.221	45.123	12.787	1.00			С
MOTA	610	CG	PHE		81	56.931	44.453	11.470	1.00			C
ATOM	611	CD1	PHE		81	57.864	43.610	10.877	1.00			C
MOTA	612	CD2	PHE		81	55.733	44.706	10.801	1.00			С
ATOM	613		PHE		81	57.614	43.027	9.631		28.62		C
ATOM	614	CE2	PHE		81	55.471	44.129	9.553	1.00			С
ATOM	615	CZ	PHE	A	81	56.414	43.290	8.969		28.84	•	C
MOTA	616	N	GLY	A	82	54.930	44.540	15.009	1.00			N
ATOM	617	CA	GLY	А	82	53.543	44.230	15.303		28.54		C
MOTA	618	C	GLY		82	52.553	45.047	14.496	1.00			С
MOTA	619	0	GLY	Α	82	51.342	44.898	14.661		28.33		0
ATOM	620	N	SER	A	83	53.068	45.914	13.629	1.00			N
MOTA	621	CA	SER	A	83	52.222	46.746	12.780	1.00	30.10		С
MOTA	622	C	SER	Α	83	51.858	45.966	11.515	1.00	30.82.		С
ATOM	623	0	SER	A	83	52.172	46.368	10.393	1.00	30.41		0
MOTA	624	CB	SER	A	83	52.947	48.046	12.423	1.00			C
MOTA	625	OG `	SER	A	83	54.228	47.778	11.889	1.00	29.80		0
ATOM	626	N	GLN	А	84	51.202	44.832	11.732	1.00	31.40		N
MOTA	627	CA	GLN	Α	84	50.752	43.941	10.674	1.00	31.71		С
MOTA	628	C	GLN	A	84	49.694	43.059	11.328	1.00	32.16		C
ATOM	629	0 .	GLN	А	84 .	49.489	43.140	12.543	1.00	32.26		0
MOTA	630	CB -	GLN	Α	84	51.915	43.093	10.147	1.00	31.73		C
MOTA	631	CG	GLN	Α	84	52.525	42.130	11.165	1.00	31.03		C
ATOM	632	CD	GLN	A	84	53.658	41.307	10.579	1.00	31.51		C
ATOM	633	OE1	GLN	Α	84	53.500	40.679	9.532	1.00	31.44		. 0
MOTA	634	NE2	GLN	A	84	54.809	41.299	11.255	1.00	30.10		N
MOTA	635	N	SER	Α	85	49.021	42.221	10.547	1.00	32.25		N
MOTA.	636	CA	SER	Α	85	47.986	41.365	11.115	1.00	32.76		C
ATOM	637	С	SER	Α	85	48.568	40.370	12.113	1.00	33.10		C
ATOM	638	0	SER	Α	85	49.736	39.988	12.020	1.00	33.02		Ó
ATOM	639	CB	SER	Α	85	47.243	40.604	10.010	1.00	32.36		C
ATOM	640	OG	SER	Α	85	48.034	39.553	9.489	1.00	32.58		0
ATOM	641	N	ILE	Α	86	47.741	39.965	13.072	1.00	33.27		N
ATOM	642	CA	ILE	A	86	48.138	39.005	14.092	1.00	33.73		C
MOTA	643	C	ILE	A	86	48.637	37.732	13.412	1.00	34.65		C
ATOM	644	0	ILE	A	86	49.670	37.167	13.785	1.00	34.09		0
ATOM	645	CB	ILE	Α	86	46.935	38.662	15.008	1.00	33.67		C
ATOM	646	CG1	ILE	А	86	46.553	39.889	15.842	1.00	33.78		C
MOTA	647	CG2	ILE	Α	86	47.267	37.479	15.898	1.00	33.45		C
MOTA	648	CD1	ILE	Α	86	45.321	39.696	16.704	1.00	34.30		C
ATOM	649	N	GLU	A	87	47.896	37.297	12.397	1.00	34.81	i	N
ATOM	650	CA	GLU	Α	87	48.235	36.093	11.650	1.00	35.57	•	C
MOTA	651	C	GLU	Α	87	49.582	36.220	10.946	1.00	34.64		C
ATOM	652	0	GLU	A	87	50.399	35.301	10.975	1.00	34.19		0
ATOM	653	CB	GLU		87	47.143	35.800	10.617	1.00	37.45		C
ATOM .	654	CG	GLU	Α	87	45.768	35.485	11.210	1.00	40.12		C
ATOM	655	CD	GLU	А	87	45.205	36.609	12.076	1.00	42.17		C
MOTA	656	OE1	GLU	Α	87	45.205	37.779	11.629	1.00	42.59		0
ATOM	657	OE2	GLU	Α	87	44.751	36.316	13.206	1.00	43.96		0
ATOM	658	N	SER	A	88	49.806	37.365	10.313	1.00	34.00		N
MOTA	659	CA	SER	Α	88	51.045	37.619	9.592	1.00	34.14		· C
MOTA	660	С	SER		88	52.264	37.630	10.523	1.00	33.33		С
ATOM	661	0	SER		88	53.291	37.015	10.225	1.00	33.84		0
MOTA	662	CB	SER		88	50.941	38.955	8.850		34.56		С
MOTA	663	OG	SER		88	52.106	39.207	8.086		37.63		0
ATOM	664	N	GLN		89	52.148	38.329	11.647		32.36		N
MOTA	665	CA	GLN		89	53.247	38.416	12.609		31.38		C.

MOTA	666	C	GLN	Α	89		53.538	37.064	13.255	1.00	31.34		С
MOTA	667	0	GLN	A	89		54.697	36.688	13.433	1.00	30.83		0
MOTA	668	CB	GLN	Α	89		52.923	39.448	13.696	1.00	30.40		C
MOTA	669	CG	GLN	Α	89		53.986	39.546	14.786		29.25		C
MOTA	670	CD	GLN	Α	89		53.629	40.544	15.877		28.00		C
MOTA	671	OE1	GLN	A	89		52.470	40.658	16.275		26.78		Ō
ATOM	672	NE2	GLN	А	89		54.632	41.258	16.378		26.79		N
MOTA	673	N	ALA	Α	90		52.486	36.333	13.608		31.60		N
ATOM	674	CA	ALA	Α	90		52.654	35.022	14.225		31.80		C
ATOM	675	C	ALA		90		53.379	34.079	13.265		32.05		C
MOTA	676	0	ALA	A	90		54.178	33.245	13.686		32.08		0
ATOM	677	СВ	ALA		90		51.297	34.447	14.613		31.91		C
MOTA	678	N	ALA	А	91		53.105	34.224	11.971		32.10	-	N
ATOM	679	CA	ALA		91	•	53.738	33.386	10.958		32.03		C
ATOM.	680	C	ALA		91		55.248	33.614	10.934		32.05		C
ATOM	681	0	ALA		91		56.026	32.666	10.818		31.83	•	
ATOM	682	СВ	ALA		91		53.137	33.678	9.578		32.23		. O
ATOM	683	N	MET		92		55.664	34.873	11.038		31.86		
ATOM '	684	CA	MET		92		57.090	35.190	11.038				N
ATOM	685	C.	MET		92		57.762	34.598		-	31.76		C
ATOM	686	0	MET		92		58.860		12.270		31.37		C
ATOM	687	СВ	MET		92			34.053	12.185		31.68		. 0
ATOM	688	CG	MET		92		57.311	36.702	11.024		31.76		C
ATOM	689	SD	MET				56.857	37.392	9.759		32.23	•	C
ATOM		CE	MET		92		57.284	39.134	9.784		32.24		S
ATOM	690				92		56.701	39.656	8.159		32.37		С
	691	N	VAL		93		57.100	34.718	13.418		31.37		N
ATOM	692	CA	VAL		93		57.639	34.185	14.667		30.84		C
MOTA	693	C	VAL		93		57.828	32.678	14.526		31.49		C
ATOM	694		VAL		93		58.901	32.142	14.805		31.13		0
ATOM	695	CB	VAL		93		56.686	34.472	15.849		30.30		C
ATOM	696		VAL		93	•	57.131	33.699	17.086	1.00	29.35		С
ATOM .	697		VAL		93		56.662	35.971	16.138	1.00	29.04		C
ATOM	698	N	HIS		94		56.775	32.003	14.076		32.42		N
ATOM	699	CA	HIS		94		56.812	30.557	13.884	1.00	33.18		С
ATOM	700	C	HIS		94		57.929	30.173	12.909	1.00	32.93		С
ATOM	701	0	HIS		94		58.667	29.217	13.147		33.48	•	0
ATOM	702	CB	HIS		94		55.447	30.078	13.369	1.00	34.65		C
MOTA	703	CG	HIS		94		55.280	28.591	13.374	1.00	35.98		C
ATOM	704		HIS		94		55.796	27.778	12.388	1.00	36.93		N
MOTA	705		HIS		94		54.656	27.768	14.251	1.00			.C
MOTA	706		HIS		94		55.497	26.519	12.657	1.00	36.90		C
ATOM	707		HIS		94		54.806	26.486	13.782	1.00	37.15		N
ATOM	708	N	ALA		95		58.067	30.928	11.823	1.00	32.80		N
ATOM	709	CA	ALA	Α	95		59.109	30.649	10.834	1.00	32.63		C
MOTA	710	C	ALA		95		60.507	30.700	11.453	1.00	32.64		С
MOTA	711	0	ALA		95		61.383	29.903	11.107	1.00	32.76		0
MOTA	712	CB	ALA	Α	95		59.019	31.641	9.677	1.00	32.50		C
MOTA	713	N	VAL	Α	96		60.721	31.642	12.365	1.00	32.04		N
ATOM	714	CA	VAL	A	96		62.023	31.770	13.011	1.00	31.47		C
MOTA	715	C	VAL	A	96		62.262	30.620	13.981	1.00	31.55		C
MOTA	716	0	VAL	A	96		63.329	30.007	13.976	1.00			0
ATOM	717	CB	VAL>	Α	96		62.142	33.105	13.783	1.00			Ċ
MOTA	718	CG1	VAL .	Α	96		63.479	33.176	14.508	1.00			C
ATOM	719	CG2	VAL .	Α	96		62.009	34.266	12.824	1.00		•	C
MOTA	720	N	LYS .	Α	97		61.261	30.327	14.805	1.00			N
ATOM	721	CA	LYS .	Α	97		61.358	29.256	15.792	1.00			C
ATOM	722	С	LYS .		97		61.543	27.872	15.169	1.00			C
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ATOM 723 O LYS A 97 62.171 26.999 15.767 1.00 34.76 ATOM 724 CB LYS A 97 59.868 30.523 17.477 1.00 31.22 ATOM 725 CG LYS A 97 59.868 30.523 17.477 1.00 31.22 ATOM 726 CD LYS A 97 61.064 30.874 18.360 1.00 29.75 ATOM 727 CE LYS A 97 61.064 30.874 18.360 1.00 29.75 ATOM 728 NZ LYS A 97 61.064 30.874 18.360 1.00 29.12 ATOM 729 N ANA 98 61.000 27.671 13.972 1.00 36.75 ATOM 730 CA ASN A 98 61.000 27.671 13.972 1.00 36.75 ATOM 731 C ASN A 98 61.000 27.671 13.972 1.00 36.75 ATOM 732 O ASN A 98 61.978 62.366 12.055 1.00 40.41 ATOM 733 CB ASN A 98 61.978 62.386 12.055 1.00 40.41 ATOM 734 CG ASN A 98 59.711 25.850 12.955 1.00 40.41 ATOM 735 ODI ASN A 98 58.468 26.461 14.912 1.00 44.16 ATOM 736 ND2 ASN A 98 58.468 26.461 14.912 1.00 41.16 ATOM 737 N PHE A 99 62.950 27.293 12.010 1.00 41.32 ATOM 739 C PHE A 99 63.837 27.410 10.854 1.00 42.24 ATOM 739 C PHE A 99 65.860 9.519 1.00 42.37 ATOM 740 O PHE A 99 65.086 29.519 1.00 42.31 ATOM 741 CB PHE A 99 65.950 27.293 12.010 1.00 42.31 ATOM 742 CG PHE A 99 65.950 27.293 12.010 1.00 42.31 ATOM 743 CD PHE A 99 65.086 29.335 8.544 1.00 42.53 ATOM 740 C PHE A 99 65.086 29.335 8.544 1.00 42.53 ATOM 740 C PHE A 99 65.086 29.335 8.544 1.00 42.53 ATOM 740 C PHE A 99 65.950 29.335 8.544 1.00 42.53 ATOM 740 C PHE A 99 65.962 29.335 8.544 1.00 42.53 ATOM 740 C PHE A 99 65.962 29.335 8.544 1.00 42.53 ATOM 740 C PHE A 99 65.962 29.335 8.544 1.00 42.53 ATOM 740 C PHE A 99 65.962 29.335 8.544 1.00 42.53 ATOM 740 C PHE A 99 65.962 29.335 8.544 1.00 42.73 ATOM 740 C PHE A 99 65.962 29.335 8.544 1.00 42.73 ATOM 740 C PHE A 99 65.962 29.335 8.644 1.00 42.73 ATOM 740 C PHE A 99 65.962 29.335 8.644 1.00 42.73 ATOM 750 C LYS A 100 66.214 22.185 11.30 1.00 42.73 ATOM 750 C LYS A 100 66.913 28.780 9.803 1.00 42.81 ATOM 750 C LYS A 100 66.924 29.566 9.803 1.00 42.81 ATOM 750 C LYS A 100 66.924 29.566 1.00 51.59 ATOM 750 C LYS A 100 66.924 29.566 1.00 51.59 ATOM 750 C LYS A 100 66.924 29.566 1.00 51.59 ATOM 750 C ALA A 101 64.125 22.202 8.666 1.00 51.59 ATOM 750 C ALA A 101 64.125 22.202 8.666 1.00 51.5		
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ATOM 773 CD2 PHE A 103 61.835 14.854 4.739 1.00 59.99 ATOM 774 CE1 PHE A 103 64.411 14.649 5.753 1.00 60.20 ATOM 775 CE2 PHE A 103 62.830 14.232 3.988 1.00 60.34 ATOM 776 CZ PHE A 103 64.122 14.130 4.497 1.00 60.26 ATOM 777 N VAL A 104 59.229 19.035 6.942 1.00 60.70 ATOM 778 CA VAL A 104 58.078 19.673 7.566 1.00 61.34		C
ATOM 774 CE1 PHE A 103 64.411 14.649 5.753 1.00 60.20 ATOM 775 CE2 PHE A 103 62.830 14.232 3.988 1.00 60.34 ATOM 776 CZ PHE A 103 64.122 14.130 4.497 1.00 60.26 ATOM 777 N VAL A 104 59.229 19.035 6.942 1.00 60.70 ATOM 778 CA VAL A 104 58.078 19.673 7.566 1.00 61.34		C
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30.704 13.235 0.324 1.00 61.90		C

ATOM	780	0	VAL	A	104	56.666	19.111	5.702	1.00 61.92		0
ATOM	781	CB	VAL	Α	104	58.185	21.212	7.479	1.00 61.42		С
ATOM	782	CG1	VAL			56.991	21.858	8.169	1.00 61.56		С
ATOM	783		VAL			59.485	21.679	8.118	1.00 61.49		С
ATOM	784	N	VAL			55.757	19.014	7.761	1.00 62.35		N
ATOM	785	CA	VAL			54.440	18.604	7.292	1.00 62.87		C
ATOM	786	C	VAL			53.715	19.808	6.697	1.00 63.08		C
ATOM	787	0	VAL			53.411	20.771	7.403	1.00 63.17		0
ATOM	788	СВ	VAL			53.591	18.034	8.450	1.00 62.93		C
ATOM	789		VAL			52.234	17.585	7.931	1.00 63.00		C
ATOM	790		VAL			54.324	16.876	9.109	1.00 62.99		C
ATOM	791	N	SER			53.445	19.751	5.397	1.00 63.19		N
ATOM	792	CA	SER			52.759	20.839	4.710	1.00 63.34		C
ATOM	793	C	SER			51.372	21.071	5.298	1.00 63.37		C
ATOM	794	0	SER			51.163	22.011	6.065	1.00 63.55		0
ATOM	795	СВ	SER			52.638	20.527	3.217	1.00 63.53		C
ATOM	796	OG	SER					2.530	1.00 63.32		0
ATOM	796 797	N	HIS			51.969 78.549	21.570 29.753	16.811	1.00 46.50		N
ATOM ·	798	CA	HIS					18.111	1.00 46.34		C
ATOM .	798 799	CA	HIS			79.214	29.762		1.00 45.34		C
ATOM	800	0	HIS			78.515 78.376	30.714 30.423	19.076 20.263	1.00 45.23		0
ATOM ·			HIS								
	801	CB				80.679	30.185	17.962	1.00 47.77		C
ATOM	802	CG ND1	HIS			81.512	29.225	17.170	1.00 49.66		C
ATOM	803		HIS			81.651	27.897	17.515	1.00 50.29		N
ATOM	804		HIS			82.269	29.406	16.061	1.00 50.09		C
ATOM	805		HIS			82.457	27.302	16.653	1.00 50.69		C
ATOM	806	NE2				82.847	28.195	15.761	1.00 50.78		N
ATOM	807	N	ASN			78.079	31.857	18.560	1.00 43.45		N
ATOM	808	CA	ASN			77.402	32.843	19.386	1.00 41.69		C
ATOM	809	C	ASN			75.906	32.910	19.120	1.00 39.79		C
ATOM		0	ASN			75.266	33.908	19.444	1.00 38.70		0
ATOM	811	CB	ASN			78.024	34.225	19.171	1.00 43.26		C
ATOM	812	CG	ASN			79.314	34.408	19.946	1.00 44.91		C
ATOM	813		ASN			79.305	34.509	21.177	1.00 45.63		0
ATOM	814		ASN			80.433	34.446	19.232	1.00 45.69		N
ATOM	815	N	GLU			75.345	31.852	18.537	1.00 37.33		N
ATOM	816	CA	GLU			73.915	31.836	18.254	1.00 35.82		C
	.817	C	GLU			73.110	31.935	19.540	1.00 33.98		C
ATOM	818.	0	GLU			73.464	31.338	20.555	1.00 34.05	•	0
ATOM	819	CB	GLU			73.508	30.560	17.499	1.00 36.85		C
ATOM	820	CG	GLU			73.919	29.250	18.173	1.00 38.61		C
ATOM	821	CD	GLU			73.188	28.035	17.613	1.00 39.59		C
ATOM	822		GLU			72.843	28.032	16.411	1.00 40.09		0
ATOM	823		GLU			72.967	27.072	18.377	1.00 40.45		0
ATOM	824	N	LEU			72.032	32.707	19.496	1.00 32.23		N
ATOM	825	CA	LEU			71.162	32.869	20.651	1.00 31.01		С
	826	C	LEU			69.988	31.928	20.443	1.00 30.52		С
ATOM	827	0			225	69.142	32.164	19.578	1.00 29.48		0
ATOM	828	CB	LEU			70.660	34.311	20.750	1.00 30.04		C
ATOM	829	CG	LEU			69.753	34.608	21.947	1.00 29.97		С
ATOM	830		LEU			70.505	34.321	23.250	1.00 29.58		С
ATOM	831		LEU			69.294	36.056	21.899	1.00 28.91		С
ATOM	832	N	VAL			69.938	30.863	21.238	1.00 30.37		N
ATOM	833	CA			226	68.874	29.875	21.107	1.00 30.90		C
ATOM	834	С			226	68.249	29.459	22.436	1.00 31.48		C
ATOM	835	0	VAL	A	226	68.767	29.782	23.512	1.00 31.51		0
ATOM	836	CB	VAL	A	226	69.405	28.604	20.414	1.00 30.86		C

ATOM	837	CG1	VAL	À	226	69.837	28.924	18.997	1.00 30.18	С
ATOM	838	CG2	VAL	Α	.226	70.579	28.040	21.209	1.00 31.20	C
ATOM	839	N	ASP	Α	227	67.130	28.743	22.352	1.00 31.82	N
ATOM	840	CA	ASP	Α	227	66.446	28.257	23.543	1.00 32.90	С
ATOM	841	C	ASP			66.961	26.857	23.874	1.00 34.23	С
ATOM	842	0	ASP			67.891	26.365	23.231	1.00 34.23	0
ATOM	843	CB	ASP			64.921	28.225	23.339	1.00 32.40	С
ATOM	844	CG	ASP			64.486	27.355	22.158	1.00 32.01	C
ATOM	845		ASP			65.177	26.369	21.829	1.00 31.77	0
ATOM	846		ASP			63.426	27.652	21.569	1.00 31.75	. 0
ATOM	847	N	SER			66.354	26.219	24.871	1.00 35.88	N
	848	CA	SER			66.767	24.881	25.289	1.00 37.61	C
ATOM ATOM	849	C			228	66.675	23.846	24.169	1.00 38.35	c
					228	67.330	22.805	24.227	1.00 38.93	Ō
ATOM	850	O					24.421	26.486	1.00 37.87	C
ATOM	851	CB			228	65.927 64.547	24.421	26.159	1.00 37.07	0
ATOM	852	OG			228			23.152	1.00 39.04	N
ATOM	853	N	GLN			65.868	24.135		1.00 39.18	C
ATOM	854	CA	GLN			65.698	23.227	22.021		C
MOTA	855	C	GLN			66.566	23.622	20.828	1.00 39.23	0
MOTA	856	0			229	66.348	23.151	19.712	1.00 39.37	
MOTA	857	CB			229	64.232	23.192	21.584	1.00 41.24	C
MOTA	858	CG			229	63.250	22.883	22.703	1.00 43.62	C
MOTA	859	CD			229	61.819	22.778	22.207	1.00 45.00	C
MOTA	860	OE1				60.871	22.836	22.992	1.00 45.95	0
ATOM	861		GLN			61.656	22.613	20.898	1.00 46.15	N
ATOM	862	N			230	67.544	24.492	21.065	1.00 38.50	N
ATOM	863	CA			230	68.451	24.949	20.013	1.00 37.74	C
ATOM	864	С			. 230	67.765	25.765	18.920	1.00 36.23	C
MOTA	865	0			230	68.303	25.921	17.824	1.00 36.06	0
MOTA	866	CB	LYS	Α	230	69.176	23.756	19.376	1.00 39.35	С
MOTA	867	CG	LYS	Α	230	70.046	22.964	20.342	1.00 41.26	С
ATOM	868	CD	LYS	A	230	71.113	23.843	20.984	1.00 43.12	С
MOTA	869	CE	LYS	A	230	71.938	23.060	21.997	1.00 44.34	C
MOTA	870	NZ	LYS	Α	230	72.907	23.933	22.723	1.00 45.01	N
MOTA	871	N	ARG	Α	231	66.579	26.283	19.217	1.00 34.84	N
ATOM	872	CA	ARG	Α	231	65.844	27.099	18.257	1.00 34.03	C
ATOM	873	C	ARG	A	231	66.203	28.565	18.499	1.00 32.95	C
ATOM	874	0	ARG	Α	231	66.289	29.001	19.646	1.00 31.96	0
ATOM	875	CB	ARG	Α	231	64.335	26.910	18.442	1.00 34.65	C
ATOM	876	CG	ARG	Α	231	63.864	25.460	18.369	1.00 35.93	C
ATOM	877	CD	ARG	Α	231	62.362	25.367	18.593	1.00 36.99	C
ATOM	878	NE	ARG	A	231	61.977	25.904	19.897	1.00 38.07	N
ATOM	879	CZ	ARG	Α	231	60.720	26.085	20.292	1.00 39.08	С
MOTA	880	NH1	ARG	Α	231	59.716	25.774	19.484	1.00 39.24	N
ATOM	881				231	60.467	26.582	21.498	1.00 40.03	N
ATOM	882	N	TYR	Α	232	66.414	29.320	17.424	1.00 31.73	N
ATOM	883	CA	TYR	Α	232	66.754	30.733	17.548	1.00 30.36	С
ATOM	884	С			232	65.701	31.473	18.364	1.00 29.68	C
ATOM	`885	0			232	64.504	31.206	18.237	1.00 28.90	0
ATOM	886	СВ			232	66.843	31.393	16.172	1.00 31.11	C
ATOM	887	CG			232	67.909	30.824	15.268	1.00 31.38	С
ATOM	888				232	69.246	30.798	15.661	1.00 31.61	С
ATOM	889				232	67.582	30.320	14.013	1.00 31.87	С
ATOM	890				232	70.233	30.279	14.820	1.00 32.53	С
ATOM	891				232	68.557	29.801	13.167	1.00 32.60	C
MOTA	892	CZ			232	69.877	29.784	13.576	1.00 32.81	С
MOTA	893	OH			232	70.838	29.280	12.730	1.00 34.16	Ō
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7 MOM	004	3.T	T THE	70	222		66 140	22 401	10 205	1.00 28.53		N
ATOM	894	N	LEU			•	66.148	32.401	19.205			
MOTA	895	CA	LEU				65.218	33.185	20.003	1.00 28.15		C
ATOM	896	С	LEU	A	233		64.666	34.306	19.136	1.00 27.30		C
MOTA	897	0	LEU	A	233		65.333	34.783	18.216	1.00 27.41		0
ATOM	898	CB	LEU	Α	233		65.913	33.801	21.224	1.00 28.49		С
ATOM	899	CG	LEU	Α	233		66.443	32.883	22.328	1.00 29.33		С
ATOM	900						66.808	33.738	23.535	1.00 29.80		С
ATOM	901		LEU				65.396	31.855	22.724	1.00 28.86		C
ATOM	902	N	VAL				63.444	34.725	19.431	1.00 26.70		N
							62.830	35.804	18.684	1.00 26.26		C
ATOM	903	CA	VAL									C
MOTA	904	C	VAL				61.821	36.512	19.564	1.00 25.94		
ATOM	905	0	VAL			`	61.172	35.892	20.407	1.00 26.26		0
MOTA	906	CB	VAL				62.120	35.288	17.407	1.00 26.74		C
ATOM	907	CG1	VAL	A	234		60.919	34.429	17.782	1.00 25.97		С
ATOM	908	CG2	VAL	А	234		61.693	36.466	16.543	1.00 25.98		С
ATOM	909	N	GLY	Α	235		61.711	37.821	19.378	1.00 25.83		N
MOTA	910	CA	GLY	Α	235		60.766	38.599	20.152	1.00 25.73		C
ATOM	911	С	GLY	Α	235		59.698	39.117	19.215	1.00 25.81		·C
ATOM	912	0	GLY				59.823	38.976	17.999	1.00 26.03		0
ATOM	913	N	ALA				58.655	39.724	19.771	1.00 25.58		N
ATOM	914	CA	ALA				57.567	40.255	18.962	1.00 24.80		C
										and the second s		C
ATOM	915	C	ALA				56.956	41.480	19.628	1.00 24.47	•	
ATOM	916	0	ALA				56.724	41.494	20.838	1.00 23.49		0
ATOM	917	CB	ALA				56.500	39.183	18.759	1.00 24.63		C
MOTA	918	N	GLY	Α	237		56.694	42.509	18.832	1.00 23.78		N
MOTA	919	CA	GLY	Α	237		56.104	43.711	19.381	1.00 23.62		C
MOTA	920	С	GLY	Α	237		54.597	43.582	19.482	1.00 24.13		C
ATOM	921	0	GLY	Α	237		53.968	42.900	18.671	1.00 23.90		0
MOTA	922	N	ILE	Α	238		54.015	44.210	20.497	1.00 24.19		N
ATOM	923	CA			238		52.570	44.188	20.654	1.00 24.84		. C
ATOM	924	C			238		52.113	45.610	20.932	1.00 25.64		c
ATOM	925	0			238		52.931	46.496	21.196	1.00 24.88		ō
	926	CB			238		52.110	43.274	21.816	1.00 24.00		C
MOTA												C
ATOM	927	CG1					52.669	43.782	23.147	1.00 24.94		
ATOM	928	CG2	ILE				52.537	41.841	21.550	1.00 24.38		C
MOTA	929	CD1	ILE				52.192	42.969	24.360	1.00 25.52		C
MOTA	930	N			239		50.807	45.831	20.854	1.00 26.34		И
ATOM	931	CA	ASN				50.251	47.147	21.116	1.00 27.12		C
MOTA	932	C	ASN	Α	239		49.239	47.032	22.248	1.00 27.64		C
MOTA	933	0	ASN	Α	239		48.820	45.932	22.610	1.00 27.63		0
ATOM	934	CB -	ASN	A	239		49.598	47.715	19.849	1.00 27.57	• 0	C
MOTA	935	CG			239			46.841	19.325			C
ATOM	936		ASN					46.731		1.00 28.35		0
ATOM	937		ASN					46.211	18.181	1.00 28.71		N
ATOM	938	N			240		48.858	48.172	22.808	1.00 28.33		N
MOTA	939	CA			240		47.916	48.210	23.916	1.00 29.57		C
		C			240					1.00 31.11		C
ATOM	940						46.456	48.037	23.496			
MOTA	941	0			240		45.553	48.160	24.324	1.00 31.21		0
MOTA	942	CB			240		48.056	49.538	24.686	1.00 29.04		C
ATOM	943		THR				47.813	50.632	23.792	1.00 29.08		0
MOTA	944	CG2	THR				49.468	49.678	25.262	1.00 27.94		С
MOTA	945	N	ARG	Α	241		46.217	47.736	22.223	1.00 32.81		N
MOTA	946	CA	ARG	A	241		44.843	47.584	21.749	1.00 34.67		С
MOTA	947	С			241		44.326	46.161	21.532	1.00 34.16		, C
MOTA	948	0			241		43.360	45.752	22.174	1.00 34.43		0
ATOM	949	CB			241			48.395	20.464	1.00 36.65		С
ATOM	950	CG			241		43.247	48.215	19.851	1.00 39.95		c
												_

MOTA	951	CD	ARG	Α	241	42.994	49.151	18.671	1.00 42.38	C
MOTA	952	NE	ARG	A	241	42.483	50.457	19.088	1.00 45.23	N
ATOM	953	CZ	ARG	A	241	43.212	51.418	19.648	1.00 46.14	C
MOTA	954	NH1	ARG	A	241	44.509	51.238	19.870	1.00 47.33	N
ATOM	955	NH2	ARG	A	241	42.642	52.566	19.990	1.00 46.48	N
ATOM	956	N	ASP	A	242	44.955	45.408	20.636	1.00 33.84	N
MOTA	957	CA	ASP	A	242	44.493	44.050	20.349	1.00 33.74	C
MOTA	958	С	ASP	A	242	45.275	42.926	21.026	1.00 33.27	C
MOTA	959	0	ASP	A	242	45.270	41.796	20.547	1.00 33.34	. 0
MOTA	960	CB	ASP	A	242	44.483	43.803	18.830	1.00 33.77	C
MOTA	961	CG	ASP	Α	242	45.874	43.869	18.206	1.00 33.91	C
MOTA	962	OD1	ASP	Α	242	46.869	43.553	18.891	1.00 34.63	0
MOTA	963	OD2	ASP	Α	242	45.975	44.220	17.012	1.00 34.44	0
MOTA	964	N	PHE	A	243	45.929	43.228	22.143	1.00 33.23	N
MOTA	965	CA	PHE	A	243	46.725	42.228	22.854	1.00 33.10	C
MOTA	966	C	PHE	Α	243	45.977	40.971	23.305	1.00 33.10	. C
MOTA	967	0	PHE	Α	243	46.553	39.883	23.330	1.00 32.90	0
MOTA	968	CB	PHE	Α	243	47.428	42.878	24.056	1.00 32.51	C
MOTA	969	CG	PHE	Α	243	46.494	43.438	25.089	1.00 31.55	C
MOTA	970	CD1	PHE	A	243	45.956	42.620	26.078	1.00 31.75	C
MOTA	971	CD2	PHE	A	243	46.155	44.785	25.077	1.00 31.51	C
ATOM	972	CE1	PHE	Α	243	45.095	43.136	27.041	1.00 31.53	Ç
ATOM	973	CE2	PHE	Α	243	45.293	45.314	26.037	1.00 31.87	C
MOTA	974	CZ	PHE	Α	243	44.763	44.487	27.022	1.00 32.20	C
MOTA	975	N	ARG	Α	244	44.703	41.104	23.660	1.00 33.75	N
MOTA	976	CA	ARG	Α	244	43.937	39.942	24.105	1.00 34.29	C
ATOM	977	C	ARG	А	244	43.920	38.850	23.042	1.00 34.39	C
MOTA	978	0	ARG	Α	244	43.801	37.666	23.355	1.00 34.22	0
MOTA	979	CB	ARG	Α	244	42.507	40.347	24.478	1.00 34.64	C
ATOM	980	CG ·			244	42.444	41.300	25.662	1.00 35.99	C
ATOM	981	CD			244	41.012	41.616	26.074	1.00 36.99	C
ATOM	982	NE			244	40.968	42.595	27.157	1.00 37.44	N
MOTA	983	CZ			244	41.260	43.884	27.012	1.00 38.60	C
ATOM	984		ARG			41.616	44.361	25.825	1.00 38.28	N
ATOM	985		ARG			41.200	44.699	28.058	1.00 39.02	N
ATOM	986	N			245	44.048	39.247	21.782	1.00 34.77	N
ATOM	987	CA			245	44.066	38.281	20.693	1.00 35.05	C
ATOM	988	C			245	45.473	38.075	20.138	1.00 34.00	C
ATOM	989	0			245	45.853	36.955	19.803	1.00 33.63	0
MOTA	990	CB			245	43.128	38.725	19.561	1.00 36.92	C
ATOM ATOM	991	CD	GLU		245	41.643	38.667	19.921	1.00 40.34	C
ATOM	992 993		GLU			41.188	39.805 39.688	20.829	1.00 42.35	C
ATOM	994		GLU			40.089 41.912	40.821	21.415 20.949	1.00 44.16 1.00 43.70	0
ATOM	995	N			246	46.249	39.151	20.949	1.00 43.70	0
ATOM	996	CA			246	47.605	39.151	19.512	1.00 32.70	N C
ATOM	997	C			246	48.569	38.278	20.403	1.00 31.03	C
ATOM	998	0			246	49.349	37.467	19.908	1.00 31.12	0
ATOM	999	СВ	ARG			48.167	40.464	19.251	1.00 30.59	C
ATOM	1000	CG			246	49.547	40.475	18.593	1.00 31.33	C
ATOM	1001	CD			246	50.027	41.901	18.325	1.00 31.90	C
ATOM	1002	NE			246	49.162	42.624	17.392	1.00 32.03	N
ATOM	1003	CZ			246	49.171	42.461	16.072	1.00 32.03	C
ATOM	1004		ARG			50.004	41.597	15.506	1.00 31.30	N
ATOM	1005		ARG			48.348	43.171	15.315	1.00 32.08	N
ATOM	1006	N	VAL			48.514	38.511	21.712	1.00 30.54	N
ATOM	1007	CA	VAL			49.411	37.822	22.638	1.00 30.81	C
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ATOM	1008	С	VAL			49.299	36.296	22.600	1.00			С
ATOM	1009	0	VAL			50.304	35.603	22.439	1.00	31.19		0
MOTA	1010	CB	VAL	Α	247	49.215	38.339	24.087	1.00	30.61		C
MOTA	1011	CG1	VAL	Α	247	49.955	37.460	25.070	1.00	29.27		C
ATOM	1012	CG2	VAL	Α	247	49.742	39.772	24.189	1.00	30.03		С
ATOM	1013	N	PRO			48.080	35.749	22.754	1.00			N
MOTA	1014	CA	PRO			47.944	34.289	22.717	1.00			C
									1.00			C
MOTA	1015	C	PRO			48.504	33.704	21.420				
ATOM	1016	0	PRO			49.142	32.650	21.421	1.00			0
ATOM	1017	CB	PRO			46.434	34.084	22.846		31.29		С
MOTA	1018	CG	PRO	A	248	46.026	35.237	23.719	1.00			C
ATOM	1019	CD	PRO	Α	248	46.802	36.388	23.118	1.00	30.24		C
ATOM	1020	N	ALA	Α	249	48.272	34.402	20.313	1.00	31.01		N
ATOM	1021	CA	ALA	Α	249	48.751	33.953	19.012	1.00	30.71		C
ATOM	1022	C	ALA	Α	249	50.277	33.926	18.960	1.00	30.92		С
ATOM	1023	0	ALA			50.871	32.989	18.421	1.00	30.39		0
ATOM	1024	CB	ALA			48.211	34.859	17.919	1.00			С
ATOM	1025	N	LEU			50.909	34.957	19.516		30.74		N
							35.035	19.521		30.84		C
ATOM	1026	CA	LEU			52.367					•	C
MOTA	1027	C	LEU			52.952	33.987	20.459		31.45		
ATOM	1028	0	LEU			53.995	33.403	20.172		31.01		0
MOTA	1029	CB	LEU			52.827	36.437	19.935		30.44		C
MOTA	1030	CG	LEU	Α	250	52.442	37.553	18.952	1.00	30.49		С
ATOM	1031	CD1	LEU	A	250	52.899	38.901	19.491	1.00	29.78		С
MOTA	1032	CD2	LEU	Α	250	53.071	37.279	17.590	1.00	29.75		С
MOTA	1033	N	VAL	Α	251	52.275	33.752	21.579	1.00	32.58		N
ATOM	1034	CA	VAL	Α	251	52.724	32.755	22.546	1.00	33.79		С
MOTA	1035	C	VAL			52.683	31.378	21.884		34.44		C
ATOM	1036	Ō	VAL			53.632	30.598	21.987		34.16		0
ATOM	1037	CB			251	51.818	32.742	23.799		34.18		Ċ
MOTA	1037		VAL			52.183	31.569	24.703		35.25		C
												C
ATOM	1039		VAL			51.965	34.055	24.554		35.24		
MOTA	1040	N			252	51.580	31.094	21.196		34.83		N
MOTA	1041	CA	GLU			51.411	29.818	20.509		35.52		C
MOTA	1042	C	GLU	A	252	52.488	29.645	19.442		34.61		C
MOTA	1043	0	GLU	Α	252	53.032	28.557	19.277	1.00	34.77		0
MOTA	1044	CB	GLU	Α	252	50.031	29.742	19.845	1.00	37.32		С
ATOM	1045	CG	GLU	A	252	49.752	28.398	19.162	1.00	40.99		C
ATOM	1046	CD	GLU	Α	252	48.561	28.429	18.203	1.00	43.11	*:	C
ATOM	1047	OE1	GLU	Α	252	48.090	27.335	17.814		44.94		. 0
ATOM	1048		GLU			48.102	29.532		1.00	44.42		0
MOTA	1049	N			253	52.784	30.723	18.719		33.41		N
ATOM	1050	CA			253	53.793	30.691	17.663		32.41		C
ATOM	1051	C	ALA			55.198	30.428	18.201		31.93		C
										31.99		0
ATOM	1052	0			253	56.104	30.078	17.441				C
MOTA	1053	CB			253	53.773	31.999			32.46		
ATOM	1054	N			254	55.384		19.504		30.81		N
MOTA	1055	CA			254	56.684	30.366	20.098		29.67		· C
MOTA	1056	C	GLY	А	254	57.527	31.587	20.431		28.80		C
ATOM	1057	0	GLY	A	254	58.723	31.452	20.686	1.00	28.19		0
MOTA	1058	N	ALA	Α	255	56.929	32.775	20.429	1.00	28.28		N
MOTA	1059	CA	ALA	Α	255	57.690	33.984	20.752	1.00	27.64		C
ATOM	1060	C.			255	58.349	33.807	22.112		27.07		C
MOTA	1061	0			255	57.721	33.341	23.059		27.00		0
ATOM	1062	CB			255	56.776	35.203	20.769		27.72		Ĉ
MOTA	1063	N			256	59.617	34.183	22.205		26.96		N
ATOM	1064	CA			256	60.368	34.049	23.446		26.98		C
TION	´T 0 0 4	CA	AOF	7	200	50.500	J4.U43	23.440	1.00	20.70		C

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ATOM.	1065	C	ASP	Α	256	60.197	35.244	24.380	1.00	26.65			C
ATOM	1066	0	ASP	Α	256	60.354	35.124	25.594	1.00	26.61			0
ATOM	1067	CB	ASP	Α	256	61.845	33.848	23.117	1.00	27.66			·C
ATOM	1068	CG	ASP	A	256	62.085	32.590	22.312	1.00	28.65			С
MOTA	1069	OD1	ASP			62.063	31.497	22.908	1.00				0
ATOM	1070		ASP			62.275	32.690	21.081	1.00				0
ATOM	1071	N	VAL			59.873	36.397	23.808	1.00				N
							37.608		1.00				C
ATOM	1072	CA	VAL			59.683		24.594					
ATOM	1073	C	VAL			58.841	38.589	23.786	1.00				C
MOTA	1074	0	VAL			58.880	38.581	22.556	1.00				0
MOTA	1075	CB	VAL			61.053	38.255	24.950	1.00				С
ATOM	1076	CG1	VAL	A	257	61.850	38.514	23.684	1.00	26.06			С
MOTA	1077	CG2	VAL	Α	257	60.847	39.550	25.725	1.00	24.98			C
ATOM	1078	N	LEU	Α	258	58.072	39.415	24.487	1.00	24.27			N
ATOM	1079	CA	LEU	Α	258	57.220	40.413	23.851	1.00	24.81			С
ATOM	1080	С	LEU	Α	258	57.652	41.801	24.319	1.00	25.12			C
MOTA	1081	0	LEU			58.377	41.936	25.304	1.00	25.19			0
ATOM	1082	CB	LEU			55.758	40.200	24.253		24.78			С
ATOM	1083	CG ·			258	55,165	38.798	24.097		25.27			C
			LEU			53.738	38.804	24.625		26.64		"	C
MOTA	1084												C
ATOM	1085					55.201	38.367	22.636		25.42			
MOTA	1086	N			259	57.202	42.829	23.612		24.79			N
MOTA	1087	CA			259	57.518	44.195	23.999		25.27			C.
ATOM	1088	C	CYS	Α	259	56.447	45.139	23.486	1.00	25.48			C
MOTA	1089	0	CYS	Α	259	56.146	45.150	22.297	1.00	25.28			0
MOTA	1090	CB	CYS	Α	259	58.883	44.628	23.448	1.00	25.05			C
MOTA	1091	SG	CYS	Α	259	59.397	46.260	24.055	1.00	24.98			S
ATOM	1092	N	ILE	Α	260	55.864	45.920	24.389	1.00	26.39			N
MOTA	1093	CA			260	54.846	46.884	23.996	1.00	27.80			C
ATOM	1094	C			260	55.571	48.017	23.275		29.01			C
ATOM	1095	Ō			260	56.492	48.627	23.816		29.15			ō
ATOM	1096	CB			260	54.108	47.462	25.210		27.85			C
										27.74			C
ATOM	1097	CG1			260	53.585	46.325	26.088					C
MOTA	1098	CG2	ILE			52.943	48.340	24.734		27.65			
MOTA	1099		ILE			52.992	46.796	27.406		29.12			C
MOTA	1100	N			261	55.136	48.287	22.054		30.05			N
MOTA	1101	CA			261	55.726	49.307	21.195		31.69			С
ATOM	1102	C			261	54.914	50.611	21.272		31.11			C
MOTA	1103	0	ASP	· A	261	53.747	50.624	20.901	1.00	31.52	÷		0
MOTA	1104	CB	ASP	Α	261	55.760	48.721	19.773	1.00	33.20			С
MOTA	1105	CG	ASP	Α	261	56.363	49.653	18.746	1.00	35.95			C
MOTA	1106	OD1	ASP	Α	261	57.279	50.427	19.080	1.00	37.14			0
ATOM	1107		ASP			55.925	49.586	17.576		37.53			0
ATOM	1108	N			262	55.524	51.692	21.769		30.51			N
MOTA	1109	CA				54.829	52.985	21.896		30.28			С
ATOM	1110	C			262	55.742	54.207	22.054		29.74			C
	1111	0			262	56.801	54.123	22.673		29.61			0
ATOM								23.087					
ATOM	1112	CB			262	53.863	52.937			31.07			C
MOTA	1113	OG			262	53.352	54.226	23.389		31.39			0
ATOM	1114	N			263	55.313	55.350	21.515		29.06			N
MOTA	1115	CA			263	56.093	56.585	21.608		28.10			С
MOTA	1116	C	SER	Α	263	56.027	57.203	23.005		27.79			C
ATOM	1117	0	SER	Α	263	56.822	58.079	23.345	1.00	28.25			0
MOTA	1118	CB	SER	A	263	55.611	57.615	20.574	1.00	28.95			С
MOTA	1119	OG	SER	Α	263	54.300	58.073	20.857	1.00	29.45			0
ATOM	1120	N			264	55.073	56.749	23.809	1.00	26.48			N
ATOM	1121	CA			264	54.923	57.245	25.173		25.78			Ċ
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MOTA	1122	С	ASP			54.400	56.107	26.043		25.45		C
MOTA	1123	0	ASP			53.191	55.891	26.144	1.00	25.07		0
MOTA	1124	CB	ASP			53.959	58.440	25.202	1.00	25.30		C
MOTA	1125	CG	ASP	A	264	53.616	58.900	26.619	1.00	24.43		C
MOTA	1126	OD1	ASP	Α	264	54.333	58.559	27.586	1.00	23.75		0
ATOM	1127	OD2	ASP	Α	264	52.618	59.629	26.760	1.00	24.33		0
ATOM	1128	N	GLY	Α	265	55.331	55.378	26.652	1.00	24.58		N
ATOM	1129	CA	GLY			54.985	54.253	27.500		24.14		С
ATOM,	1130	C	GLY			54.505	54.603	28.896		24.38		Ċ
ATOM	1131	0	GLY			54.105	53.718	29.655		23.84		0
ATOM	1132	N	PHE			54.554	55.884	29.250		24.38		N
ATOM	1133	CA	PHE			54.095	56.321	30.562		24.40		C
ATOM	1134	C	PHE			52.584	56.429	30.382		24.85		C
MOTA	1135	0	PHE			52.035	57.523	30.275		23.66		0
ATOM	1136	CB	PHE			54.700	57.685	30.902		24.77		C
MOTA	1137	CG	PHE			54.758	57.987	32.383	1.00	25.09		С
MOTA	1138	CD1	PHE	Α	266	54.030	57.233	33.302	1.00	24.80		C
ATOM	1139	CD2	PHE	Α	266	55.530	59.047	32.851	1.00	24.88		С
ATOM	1140	CE1	PHE	Α	266	54.071	57.533	34.665	1.00	25.40		C
MOTA	1141	CE2	PHE	Α	266	55.580	59.360	34.210	1.00	24.97		С
ATOM	1142	CZ	PHE			54.849	58.601	35.121	1.00	25.68		C.
ATOM	1143	N	SER			51.924	55.274	30.348		25.48		N
ATOM	1144	CA	SER			50.486	55.203	30.112		26.23		C
ATOM	1145	C	SER			49.777	54.078	30.855		26.64		c
ATOM	1145	0	SER			50.306	52.971	30.983		25.99		0
ATOM	1147	CB	SER			50.241	55.016	28.616		26.26		C
ATOM	1148	OG	SER			48.898	54.647	28.356		28.51		0
ATOM	1149	N	GLU			48.567	54.363	31.321		27.32	,	N
MOTA	1150	CA	GLU			47.776	53.363	32.021		28.41		C
MOTA	1151	С	GLU			47.486	52.195	31.089		28.35		C
MOTA	1152	0 ,	GLU	Α	268	47.276	51.070	31.544	1.00	27.34		0
MOTA	1153	CB	GLU	Α	268	46.454	53.964	32.513	1.00	30.40		C
ATOM	1154	CG	GLŪ	A	268	46.594	54.834	33.754	1.00	33.77		C
MOTA	1155	CD	GLU	Α	268	45.255	55.298	34.320	1.00	35.87		C
ATOM	1156	OE1	GLU	Α	268	45.246	55.792	35.471	1.00	37.72		0
ATOM	1157	OE2	GLU	A	268	44.221	55.177	33.623	1.00	35.03		0
ATOM	1158	Ñ	TRP	Α	269	47.471	52.464	29.785	1.00	28.35	•	N
MOTA	1159	CA	TRP			47.204	51.417	28.806	1.00	29.40		C
ATOM	1160	C	TRP			48.275	50.332	28.857		29.06		C
ATOM	1161	0	TRP			47.976	49.154	28.653		29.12		Ö
ATOM	1162	CB	TRP			47.121	51.995	27.388		30.30		C
ATOM	1163	CG	TRP			45.916	52.861	27.150		32.00		C
			TRP			45.908				32.39		
MOTA	1164						54.202	26.892				C
ATOM	1165		TRP			44.543	52.443	27.146		32.75		C
ATOM	1166		TRP			44.617	54.644	26.727		33.20	•	N
MOTA	1167		TRP			43.760	53.586	26.877		33.15		C
ATOM	1168		TRP			43.899	51.212	27.343		33.57		C
ATOM	1169				269.	42.363	53.539	26.798		33.93		С
MOTA	1170					42.507	51.164	27.266	1.00	34.42		C
ATOM	1171	CH2	TRP			41.757	52.323	26.994	1.00	34.51		C
MOTA	1172	N	${\tt GLN}$	Α	270	49.519	50.726	29.122	1.00	28.51		N
MOTA	1173	CA	GLN	Α	270	50.610	49.755	29.209	1.00	28.61		С
ATOM	1174	С	GLN			50.460	48.941	30.490		28.10		С
ATOM	1175	0	GLN			50.699	47.736	30.499		28.60		0
ATOM	1176	СВ	GLN			51.977	50.457	29.205		28.36		Ċ
ATOM	1177	CG	GLN			52.238	51.315	27.977		28.23		C
ATOM	1178	CD	GLN			53.519	50.943	27.244		28.01		C
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ATOM	1179	OE1	GLN	Α	270	54.445	50.374	27.825	1.00 27.19		0
ATOM	1180	NE2	GLN	Α	270	53.581	51.282	25.963	1.00 26.48		N
MOTA	1181	N	LYS	Α	271	50.072	49.604	31.575	1.00 28.37		N
ATOM	1182	CA	LYS	Α	271	49.878	48.915	32.846	1.00 28.70		С
ATOM	1183	C	LYS	Α	271	48.784	47.858	32.671	1.00 27.88		C
ATOM	1184	0	LYS			48.917	46.734	33.144	1.00 27.93		0
ATOM	1185	СВ	LYS			49.476	49.912	33.941	1.00 29.92		C
						49.092	49.260	35.266	1.00 32.48		C
ATOM	1186	CG	LYS						1.00 34.72		C
ATOM	1187	CD	LYS			48.701	50.309	36.300			C
MOTA	1188	CE	LYS			48.207	49.671	37.590	1.00 36.23		
MOTA	1189	NZ	LYS			49.269	48.881	38.274	1.00 38.61		N
MOTA	1190	N	ILE			47.712	48.231	31.979	1.00 27.39		N
ATOM	1191	CA	ILE	A	272	46.592	47.326	31.726	1.00 27.48		C
MOTA	1192	С	ILE	Α	272	47.036	46.124	30.902	1.00 26.99		С
ATOM	1193	0	ILE	Α	272	46.668	44.989	31.195	1.00 27.02		0
ATOM	1194	CB	ILE	A	272	45.447	48.057	30.978	1.00 27.22		C
MOTA	1195	CG1				44.786	49.064	31.922	1.00 27.67		С
ATOM	1196	CG2				44.422	47.046	30.447	1.00 27.76		C
ATOM	1197	CD1				43.836	50.030	31.231	1.00 27.85		С
ATOM	1198	N			273	47.831	46.377	29.868	1.00 26.65		N
							45.306	29.010	1.00 26.53		C
ATOM	1199	CA			273	48.322				•	C
MOTA	1200	C			273	49.202	44.331	29.792	1.00 26.14		
MOTA	1201	0			273	49.041	43.114	29.694	1.00 25.79		0
MOTA	1202	CB			273 .	49.120	45.878	27.824	1.00 26.74		Ċ
ATOM	1203	OG1	THR	A	273	48.270	46.744	27.059	1.00 27.53		0
MOTA	1204	CG2	THR	Α	273	49.626	44.752	26.928	1.00 27.26		C
ATOM	1205	N	ILE	Α	274	50.134	44.863	30.571	1.00 26.20		N
MOTA	1206	CA	ILE	Α	274	51.010	44.003	31.357	1.00 26.20	•	С
MOTA	1207	С	ILE	Α	274	50.175	43.230	32.377	1.00 26.66		C
ATOM	1208	0			274	50.411	42.045	32.616	1.00 26.11		0
ATOM	1209	CB			274	52.080	44.821	32.096	1.00 25.86		С
ATOM	1210	CG1			274	52.942	45.581	31.082	1.00 26.16		С
	1211	CG2		•	274	52.950	43.895	32.945	1.00 25.61		C
ATOM			ILE			53.895	46.583	31.715	1.00 27.00		C
MOTA	1212							32.966	1.00 26.98		N
ATOM	1213	N			275	49.194	43.908				C
MOTA	1214	CA			275	48.335	43.266	33.949	1.00 28.29		
MOTA	1215	C			275	47.599	42.064	33.382	1.00 28.55		C
MOTA	1216	0			275	47.537	41.009	34.015	1.00 28.98		0
MOTA	1217	N			276	47.041	42.222	32.187	1.00 28.87		N
MOTA	1218	CA	TRP	Α	276	46.312		31.526	1.00 28.90		C
ATOM	1219	C	TRP	Α	276	47.246	39.963	31.270	1.00 29.40	•	C
MOTA	1220	0	TRP	Α	276	46.864	38.802	31.453	1.00 29.24		0
MOTA	1221	CB	TRP	Α	276	45.735	41.633	30.197	1.00 29.68		C
ATOM	1222	CG	TRP	Α	276	44.847	40.631	29.531	1.00 30.48		C
ATOM	1223	CD1	TRP			43.513	40.429	29.766	1.00 30.71		С
ATOM	1224				276	45.230	39.673	28.539	1.00 30.72		С
ATOM	1225				276	43.043	39.405	28.977	1.00 30.48		N
ATOM	1226				276	44.075	38.922	28.214	1.00 31.35		С
ATOM	1227				276	46.437	39.373	27.891	1.00 31.18		C
							37.890	27.268	1.00 31.27		C
ATOM	1228				276	44.092			1.00 31.27		C
ATOM	1229				276	46.455	38.344	26.951			
MOTA	1230				276	45.287	37.616	26.649	1.00 31.77		C
ATOM	1231	N			277	48.472	40.256	30.844	1.00 28.84		N
MOTA	1232,	CA			277	49.440	39.197	30.585	1.00 28.97		C
MOTA	1233	С	ILE	A	277	49.774	38.442	31.878	1.00 29.36		C
MOTA	1234	0	ILE	Α	277	49.822	37.213	31.886	1.00 28.83		0
MOTA	1235	CB	ILE	Α	277	50.740	39.765	29.950	1.00 28.28		C

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MOTA	1236	CG1	ILE	Α	277		50.442	40.296	28.542	1.00 28.37		С
MOTA	1237	CG2	ILE	Α	277		51.802	38.678	29.867	1.00 28.02		C
ATOM	1238	CD1	ILE				51.604	41.054	27.890	1.00 27.79		С
MOTA	1239	N	ARG				49.988	39.174	32.969	1.00 30.21		N
MOTA	1240	CA	ARG	Α	278		50.312	38.551	34.254	1.00 31.53		С
MOTA	1241	С	ARG	Α	278		49.173	37.683	34.776	1.00 33.21		C
MOTA	1242	0	ARG	Α	278		49.400	36.609	35.334	1.00 33.46		0
MOTA	1243	CB	ARG	Α	278		50.643	39.616	35.304	1.00 30.82		С
ATOM	1244	CG	ARG	А	278		51.957	40.335	35.071	1.00 30.23		С
MOTA	1245	CD	ARG	Α	278		53.143	39.393	35.206	1.00 29.99		С
MOTA	1246	NE	ARG	A	278		54.382	40.066	34.832	1.00 28.97		N
MOTA	1247	CZ	ARG				55.148	39.711	33.806	1.00 28.64		C
MOTA	1248		ARG				54.812	38.677	33.044	1.00 26.58		N
MOTA	1249	NH2	ARG				56.243	40.409	33.530	1.00 27.89		N
ATOM	1250	N			279		47.949	38.168	34.597	1.00 34.74		N
ATOM	1251	CA			279		46.754	37.466	35.043	1.00 36.51		C
MOTA	1252	C	GLU				46.553	36.166	34.268	1.00 36.74		С
ATOM	1253	0			279		46.101	35.162	34.819	1.00 36.85		0
MOTA	1254	CB	GLU				45.541	38.384	34.859	1.00 38.13		C
MOTA	1255	CG			279		44.204	37.819	35.314	1.00 41.43		C
MOTA	1256	CD			279		43.065	38.828	35.182	1.00 43.32	-	C
	1257	OE1	GLU				41.902	38.449	35.442	1.00 44.56		0
MOTA	1258		GLU				43.327	40.002	34.823	1.00 44.56	•	0
MOTA	1259	N	LYS				46.915	36.183	32.991	1.00 36.37		N
ATOM	1260	CA	LYS				46.742	35.019	32.133	1.00 36.81		C
MOTA	1261	C			280		47.941	34.071	32.107	1.00 36.04		C
MOTA	1262	0	LYS				47.773	32.854	32.038	1.00 35.58		0
MOTA	1263	CB			280		46.433	35.495	30.710	1.00 38.33		C
MOTA	1264	CG			280		45.519	34.591	29.895	1.00 40.96		C
MOTA	1265	CD			280		46.185	33.281	29.512	1.00 42.35		C
ATOM	1266	CE	LYS				45.280	32.456	28.601	1.00 42.90		C
ATOM	1267	NZ			280	*	44.954	33.184	27.341	1.00 42.89		N
MOTA	1268	N			281		49.146	34.627	32.185	1.00 34.52		N
ATOM	1269	CA			281		50.362	33.826	32.100	1.00 33.39		C
ATOM ATOM	1270	С О			281		51.328	33.919	33.274	1.00 33.09		C
ATOM	1271 1272	CB			281 281		52.334	33.214	33.297 30.834	1.00 33.09 1.00 32.75		0
ATOM	1272	CG			281		51.124	34.209	29.549	1.00 32.75		C
ATOM	1273	CD1	TYR				50.356 50.221	34.016	28.976	1.00 32.31		C
MOTA	1275	CD2					49.785	32.752 35.103	28.889	1.00 32.30		C
ATOM	1276				281		49.763	32.577	27.774	1.00 32.48	*	C
ATOM	1277		TYR				49.104	34.939	27.691	1.00 32.47		C
ATOM	1278	CZ			281		48.987	33.674	27.138	1.00 32.49		C
ATOM	1279	OH			281		48.328	33.512	25.941	1.00 33.37		o
ATOM	1280	N			282		51.043	34.780	34.240	1.00 33.37		N
ATOM	1281	CA			282		51.961	34.919	35.355	1.00 32.77		C
ATOM	1282	C			282		53.284	35.449	34.826	1.00 33.10		C
MOTA	1283	Ō			282		53.305	36.220	33.863	1.00 32.17		0
ATOM	1284	N			283		54.391	35.041	35.436	1.00 33.13		N
ATOM	1285	CA			283		55.699	35.501	34.986	1.00 33.88		C
ATOM	1286	C			283		56.322	34.574	33.945	1.00 33.49		C
ATOM	1287	Ō			283		57.519	34.647	33.674	1.00 34.01		0
ATOM	1288	СВ			283		56.637	35.665	36.184	1.00 34.83		C
ATOM	1289	CG			283		56.242	36.833	37.072	1.00 36.88		C
ATOM	1290		ASP				56.206	37.978	36.569	1.00 38.24		ō
ATOM	1291		ASP				55.965	36.615	38.270	1.00 38.21		Ō
MOTA	1292	N			284		55.504	33.711	33.352	1.00 33.24		N

MOTA	1293	CA	LYS	A	284	55.985	32.773	32.342	1.00	33.02			С
MOTA	1294	C .	LYS	Α	284	56.118	33.426	30.968	1.00	32.02			С
MOTA	1295	0	LYS	А	284	56.838	32.931	30.105	1.00	32.97			0
MOTA	1296	CB	LYS	А	284	55.058	31.551	32.275	1.00	34.39			С
MOTA	1297	CG	LYS	Α	284	55.260	30.568	33.433	1.00	36.82			C
MOTA	1298	CD	LYS	Α	284	55.284	31.281	34.783	1.00	38.42			С
MOTA	1299	CE	LYS	A	284	55.742	30.359	35.910	1.00	39.93	•		C
MOTA	1300	NZ	LYS	A	284	56.028	31.120	37.168	1.00	39.68			N
MOTA	1301	N	VAL	Α	285	55.410	34.530	30.761	1.00 2	29.89			N
MOTA	1302	CA	VAL	A	285	55.510	35.259	29.502	1.00 2	28.50			C
MOTA	1303	C	VAL	Α	285	56.233	36.566	29.813 ⁻	1.00 2				C
MOTA	1304	0	VAL	A	285	55.816	37.326	30.691	1.00 2	27.10			0
MOTA	1305	CB	VAL	А	285	54.122	35.559	28.895	1.00 2	28.58			С
MOTA	1306	CG1	VAL	Α	285	54.259	36.563	27.748	1.00 2	27.74			C
MOTA	1307	CG2	VAL	A	285	53.502	34.264	28.375	1.00 2				С
MOTA	1308	N	LYS	Α	286	57.327	36.815	29.101	1.00 2				N
ATOM	1309	CA	LYS	A	286	58.125	38.014	29.317	1.00	24.52		Θ.	С
MOTA	1310	С	LYS	А	286	57.671	39.148	28.410	1.00	24.47			C
MOTA	1311	0	LYS	A	286	57.419	38.944	27.222	1.00	24.28			Ò.
ATOM	1312	CB ·	LYS.	·Α	286	59.601	37.697	29.076	1.00	25.16			С
ATOM	1313	CG	LYS	A	286	60.112	36.510	29.893	1.00	24.27			С
MOTA	1314	CD	LYS	Α	286	59.926	36.746	31.388	1.00	24.81			С
ATOM	1315	CE	LYS	Α	286	60.396	35.544	32.204	1.00	25.83			C
MOTA	1316	NZ	LYS	A	286	60.194	35.749	33.670	1.00	24.86			N
MOTA	1317	N	VAL	A	287	57.574	40.347	28.972	1.00	24.27			N
MOTA	1318	CA	VAL	A	287	57.120	41.495	28.202	1.00	24.13		-	С
MOTA	1319	С	VAL	Α	287	57.779	42.813	28.597	1.00	23.84	•		C
MOTA	1320.	0	VAL	Α	287	57.687	43.255	29.743	1.00	23.87			0
MOTA	1321	CB	VAL	A	287	55.573	41.644	28.308	1.00	24.31			С
ATOM	1322	CG1	VAL	A	287	55.146	41.662	29.769	1.00	25.02			С
MOTA	1323	CG2	VAL	A	287	55.114	42.923	27.609	1.00	24.49			C
MOTA	1324	N	GLY	A	288	58.456	43.428	27.634	1.00	23.20			N
ATOM	1325	CA	GLY	Α	288	59.097	44.707	27.882	1.00	22.85			C
MOTA	1326	C	GLY	A	288	58.077	45.801	27.643	1.00	22.44			С
MOTA	1327	0	GLY	Α	288	57.018	45.548	27.063	1.00	22.27			0
ATOM	1328	N	ALA	A	289	58.383	47.014	28.088	1.00	22.59			И
MOTA	1329	CA	ALA	Α	289	57.468	48.139	27.922	1.00	23.01			С
MOTA	1330	C	ALA	A	289	58.248	49.422	27.682	1.00	23.15			С
MOTA	1331	Ο.	ALA	A	289	59.438	49.498	27.976	1.00				0
MOTA	1332	CB	ALA	А	289	56.573	48.287	29.168	1.00	23.19			C
MOTA	1333	N	GLY	А	290	57.565	50.427	27.144	1.00				N
MOTA	1334	CA	GLY	Α	290	58.205	51.698	26.856	1.00	23.22			С
MOTA	1335	C	GLY	A	290	57.432	52.435	25.775	1.00				C
MOTA	1336	0	GLY	Α	290	56.397	51.945	25.320	1.00				0
ATOM	1337	N	ASN	Α	291	57.937	53.582	25.324	1.00				N
MOTA	1338	CA	ASN	Α	291	59.199	54.155	25.787	1.00	22.55			С
MOTA	1339	C			291	59.028	55.263	26.817	1.00				С
MOTA	1340	0			291	58.024	55.974	26.817	1.00				0
ATOM	1341	CB			291	59.977	54.727	24.592	1.00				С
ATOM	1342	CG	ASN	Α	291	60.565	53.651	23.708	1.00	22.60			С
MOTA	1343		ASN			60.148	52.493	23.758	1.00				0
MOTA	1344	ND2	ASN	A	291	61.538	54.029	22.884	1.00				N
MOTA	1345	N			292	60.028	55.404	27.685	1.00				N
MOTA	1346	CA			292	60.031	56.448	28.702	1.00				C
ATOM	1347	C			292	61.391	57.144	28.669	1.00				C
MOTA	1348	0			292	62.327	56.651	28.033	1.00				0
MOTA	1349	CB	ILE	A	292	59.722	55.879	30.123	1.00	22.99			С

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ATOM	1350		ILE			60.591	54.655	30.437	1.00 22.90		С
MOTA	1351	CG2	ILE			58.243	55.506	30.208	1.00 23.43		С
ATOM	1352	CD1	ILE			62.040	54.972	30.767	1.00 23.93		C
MOTA	1353	N	VAL			61.502	58.296	29.322	1.00 22.08		N
MOTA	1354	CA	VAL			62.765	59.028	29.320	1.00 22.29		С
ATOM	1355	C	VAL			63.201	59.555	30.678	1.00 22.70		C
MOTA	1356	0	VAL	A	293	64.187	60.282	30.766	1.00 22.85		0
MOTA	1357	CB	VAL	A	293	62.720	60.228	28.346	1.00 22.95		С
ATOM	1358	CG1	VAL	Α	293	62.595	59.730	26 . 906	1.00 22.15		C
MOTA	1359	CG2	VAL	Α	293	61.550	61.148	28.706	1.00 22.40		С
ATOM	1360	N	ASP	Α	294	62.474	59.209	31.736	1.00 22.82		N
ATOM	1361	CA	ASP	А	294	62.851	59.680	33.060	1.00 23.34		C
MOTA	1362	C	ASP	A	294 .	62.532	58.660	34.145	1.00 23.54		С
ATOM	1363	0	ASP	A	294	61.897	57.634	33.880	1.00 23.02		0
ATOM	1364	CB	ASP	А	294	62.181	61.040	33.365	1.00 23.61		С
ATOM	1365	CG	ASP			60.680	60.934	33.635	1.00 24.61		C
ATOM	1366	OD1	ASP			60.057	59.898	33.323	1.00 25.36		0
ATOM	1367		ASP			60.115	61.921	34.158	1.00 24.53		0
ATOM	1368		GLY			62.991	58.943		1.00 23.57	٠.	N
ATOM	1369	CA	GLY			62.762	58.043	36.474	1.00 24.71		C
ATOM	1370	C	GLY			61.300	57.752	36.756	1.00 24.99		C
ATOM	1371	0	GLY			60.943	56.611	37.038	1.00 24.55		ō
ATOM	1372	N	GLU			60.455	58.777	36.692	1.00 25.66		N
ATOM	1373	CA	GLU			59.022	58.603	36.943	1.00 26.31		C
ATOM	1374	C	GLU			58.413	57.575	36.001	1.00 25.52		C
ATOM	1375	0	GLU			57.635	56.715	36.421	1.00 24.66		0
ATOM	1376	CB	GLU			58.269	59.924	36.759	1.00 24.00		C
ATOM	1377	CG							1.00 33.07		C
		CD	GLU			58.342	60.889	37.927	1.00 33.07		C
MOTA	1378		GLU			57.642	62.208	37.621			
MOTA	1379	OE1	GLU			56.485	62.181	37.130	1.00 37.36		0
MOTA	1380	OE2				58.250	63.272	37.871	1.00.38.01		0
MOTA	1381	N			297	58.750	57.687	34.721	1.00 25.01		N
ATOM	1382	CA	GLY			58.227	56.761	33.733	1.00 24.76		C
ATOM	1383	C	GLY			58.735	55.353	33.981	1.00 24.56		C
ATOM	1384	0	GLY			57.976	54.384	33.891	1.00 24.54		0
ATOM	1385	N	PHE			60.026	55.238	34.279	1.00 23.53		И
ATOM	1386	CA	PHE			60.628	53.938	34.559	1.00 23.73		C
ATOM	1387	C			298	59.904	53.288	35.737	1.00 23.95		C
MOTA	1388	0.			298	59.470	52.140		1.00 23.92		0
ATOM	1389	CB	PHE			62.107	54.091	34.926	1.00 22.70		C
ATOM	1390	CG	PHE			62.710	52.844	35.510	1.00 22.74		C
MOTA	1391		PHE			63.206	51.841	34.685	1.00 22.49		C
MOTA	1392		PHE			62.702	52.636	36.885	1.00 22.82		C
ATOM	1393		PHE			63.680	50.645	35.223	1.00 22.80		C
MOTA	1394	CE2	PHE			63.171	51.447	37.433	1.00 22.71		C
MOTA	1395	CZ	PHE			63.659	50.448	36.599	1.00 22.47		C
ATOM	1396	N	ARG	A	299	59.800	54.043	36.829	1.00 24.49		N
MOTA	1397	CA	ARG	Α	299	59.158	53.588	38.062	1.00 25.88		С
MOTA	1398	C	ARG	А	299	57.736	53.090	37.833	1.00 25.06		С
ATOM	1399	0	ARG	A	299	57.323	52.074	38.402	1.00 24.51		0
MOTA	1400	CB	ARG	Α	299	59.154	54.735	39.080	1.00 28.63		Ç
MOTA	1401	CG	ARG	Α	299	58.300	54.510	40.313	1.00 32.44		С
MOTA	1402	CD	ARG	A	299	59.044	53.764	41.400	1.00 35.12		C
MOTA	1403	NE	ARG	A	299	60.302	54.414	41.772	1.00 37.30		N
ATOM	1404	CZ	ARG	A	299	61.032	54.061	42.827	1.00 37.36		С
MOTA	1405	NH1	ARG	Α	299	60.620	53.077	43.614	1.00 37.31		N
ATOM	1406		ARG			62.186	54.665	43.079	1.00 37.90		N

MOTA	1407	N	TYR	A	300	56.987	53.804	36.998	1.00 23.80	N
MOTA	1408	CA			300	55.615	53.413	36.717	1.00 23.18	C
MOTA	1409	С	TYR	A	300	55.549	52.050	36.022	1.00 22.98	C
MOTA	1410	0			300	54.760	51.189	36.405	1.00 22.25	0
ATOM	1411	CB	TYR	A	300	54.929	54.460	35.837	1.00 23.21	C
MOTA	1412	CG	TYR	Α	300	53.474	54.153	35.573	1.00 23.56	C
MOTA	1413	CD1	TYR	Α	300	52.505	54.362	36.560	1.00 24.05	. C
MOTA	1414	CD2	TYR	A	300	53.066	53.632	34.349	1.00 23.81	С
MOTA	1415	CE1	TYR	A	300	51.164	54.059	36.325	1.00 24.38	С
MOTA	1416	CE2	TYR	Α	300	51.734	53.325	34.105	1.00 24.00	C
MOTA	1417	CZ	TYR	Α	300	50.790	53.540	35.094	1.00 23.95	C
MOTA	1418	OH	TYR	A	300	49.474	53.239	34.845	1.00 24.48	0
ATOM	1419	N	LEU	Α	301	56.372	51.857	34.996	1.00 21.97	N
MOTA	1420	CA			301	56.366	50.592	34.274	1.00 22.14	С
MOTA	1421	C	LEU	Α	301	56.991	49.463	35.102	1.00 22.14	C
MOTA	1422	Ò	LEU	Α	301	56.625	48.298	34.947	1.00 22.36	0
ATOM	1423	CB	LEU	Α	301	57.081	50.741	32.920	1.00 21.32	· C
ATOM	1424	CG	LEU	Α	301	56.381	51.668	31.909	1.00 21.51	С
ATOM	1425	CD1	LEU	Α	301	57.204	51.757	30.618	1.00 21.05	C
ATOM	1426	CD2	LEU	Α	301	54.972	51.136	31.607	1.00 21.05	С
ATOM	1427	N	ALA	Α	302	57.925	49.808	35.984	1.00 22.39	N
MOTA	1428	CA	ALA			58.559	48.799	36.833	1.00 23.49	C
MOTA	1429	С	ALA			57.500	48.240	37.790	1.00 24.06	С
MOTA	1430	0	ALA	A	302	57.357	47.022	37.937	1.00 23.67	0
ATOM	1431	CB	ALA			59.708	49.415	37.625	1.00 22.59	C
MOTA	1432	N	ASP			56.760	49.138	38.432	1.00 24.53	N
MOTA	1433	CA	ASP			55.709	48.734	39.360	1.00 26.12	C
MOTA	1434	C	ASP			54.589	48.010	38.614	1.00 26.16	C
MOTA	1435	0	ASP			53.891	47.179	39.194	1.00 26.12	, 0
MOTA	1436	CB	ASP			55.121	49.948	40.094	1.00 27.14	C
ATOM	1437	CG	ASP			56.086	50.560	41.103	1.00 28.94	С
MOTA	1438		ASP			56.998	49.856	41.586	1.00 30.42	. 0
MOTA	1439	OD2	ASP			55.916	51.751	41.432	1.00 30.69	0
ATOM	1440	N	ALA			54.416	48.333	37.332	1.00 25.47	N.
ATOM	1441	CA	ALA			53.386	47.695	36.517	1.00 25.15	C
ATOM	1442	С	ALA			53.755	46.246	36.196	1.00 25.19	C
ATOM	1443	0	ALA			52.895	45.451	35.811	1.00 24.86	0
MOTA	1444	СВ	ALA			53.172	48.472	35.233	1.00 24.93	C
ATOM	1445	N	GLY			55.035	45.909	36.337	1.00 24.65	N
ATOM	1446	CA	GLY			55.461	44.540	36.086	1.00 24.64	C
ATOM	1447	C	GLY			56.306	44.266	34.851	1.00 24.36	C
ATOM	1448	0	GLY			56.597	43.107	34.547	1.00 24.74	. 0
ATOM	1449	N	ALA			56.711	45.311	34.140	1.00 23.62	N
ATOM	1450	CA	ALA			57.521	45.136	32.935	1.00 23.66	C
ATOM	1451	C	ALA			58.803	44.351	33.214	1.00 23.20	C
ATOM	1452	0	ALA			59.430	44.532	34.256	1.00 23.66	0
ATOM	1453	CB	ALA			57.866	46.499	32.336	1.00 22.87	C
ATOM	1454	N	ASP			59.188	43.490	32.274	1.00 23.16	N
ATOM	1455	CA	ASP			60.398	42.679	32.406	1.00 22.69	C
MOTA	1456	C	ASP			61.659	43.439	31.998	1.00 22.59	C
ATOM	1457	0	ASP			62.764	43.098	32.415	1.00 22.56	0
ATOM	1458	CB	ASP			60.243	41.391	31.601	1.00 23.45	С
ATOM	1459	CG	ASP			59.292	40.424	32.267	1.00 23.60	C
ATOM ATOM	1460		ASP			59.626	39.963	33.375	1.00 24.19	. 0
ATOM	1461		ASP			58.217	40.144	31.705	1.00 23.04	. 0
ATOM	1462 1463	N Ch	PHE			61.482	44.453	31.159	1.00 22.02	N
AION	1402	CA	PHE	А	308	62.571	45.334	30.756	1.00 21.84	C

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MOTA	1464	С	PHE	A	308		61.903	46.608	30.264	1.00	21.93			C
ATOM	1465	0	PHE	A	308		60.755	46.587	29.809	1.00	20.69			0
MOTA	1466	CB	PHE	A	308		63.505	44.695	29.700	1.00	21.68			C
MOTA	1467	CG	PHE	A	308		62.928	44.596	28.312	1.00	22.97			С
ATOM	1468	CD1	PHE	A	308		62.892	45.707	27.470	1.00	23.01			С
ATOM	1469	CD2	PHE	Α	308		62.487	43.369	27.820	1.00	22.89			C
ATOM	1470	CE1	PHE	Α	308		62.431	45.596	26.153	1.00	23.45			С
MOTA	1471	CE2	PHE	A	308		62.023	43.245	26.504		23.97	•		С
ATOM	1472	CZ	PHE	A	308		61.998	44.362	25.669		23.35			C
MOTA	1473	N	ILE				62.609	47.724	30.381		20.99			N
MOTA	1474	CA	ILE	A	309		62.040	49.001	29.994		21.61			С
ATOM	1475	С	ILE				62.877	49.704	28.929		21.29			C.
MOTA	1476	0			309		64.096	49.835	29.071		20.03			0
MOTA	1477	CB	ILE				61.866	49.881	31.264		21.66			С
ATOM	1478	CG1					60.841	49.204	32.189		22.00			C
MOTA	1479	CG2	ILE				61.444	51.298	30.886		20.92			C
ATOM	1480	CD1	ILE				60.725	49.797	33.575		22.70			С
ATOM	1481	N	LYS				62.212	50.132	27.854		21.58			N
MOTA	1482	CA	LYS				62.884	50.809	26.745		21.98			C
MOTA	1483	C	LYS				62.919	52.317	26.942		21.74			C
ATOM	1484	0	LYS			-	61.907	52.942	27.271		21.19			0
ATOM	1485	CB	LYS				62.211	50.489	25.404		23.35			C
ATOM	1486	CG	LYS				62.440	49.071	24.915		26.33			C
ATOM	1487	CD	LYS				62.448	48.987	23.377		24.86			C
ATOM	1488	CE	LYS				61.072	49.221	22.764		26.09			C
MOTA	1489	NZ	LYS				60.922	50.568	22.124		25.19			N
ATOM	1490	N			311		64.093	52.890	26.704		20.80			И
ATOM	1491	CA			311		64.330	54.319	26.888		20.47			С
ATOM	1492	C			311		64.496	55.076	25.578		20.59			С О
MOTA	1493	O			311		65.258	54.658	24.707		20.84			C
MOTA	1494	CB			311		65.625	54.543 53.813	27.695 29.039		19.79			C
ATOM ATOM	1495 1496	CG1 CG2	ILE		311		65.544 65.876	56.037	27.885		19.52			C
ATOM	1490	CD1			311		66.917	53.602	29.686		19.29			C
ATOM	1497	N			312	•	63.796	56.197	25.444		21.35			N
ATOM	1499	CA			312		63.962	56.992	24.247		22.14			C
ATOM	1500	C			312		62.738	57.526	23.542		22.59			C
ATOM	1501	0			312		61.877	56.771	23.106		22.49			ō
ATOM	1502	N			313		62.670	58.847	23.430		23.41			N
ATOM	1503	CA			313		61.577	59.497	22.725		24.56			C
ATOM	1504	C			313		62.156	60.654	21.912		25.54			Ċ
MOTA	1505	0			313		62.786	61.553	22.467		24.97		*	ō
MOTA	1506	CB			313		60.505	60.047	23.692		24.81			Ċ
ATOM	1507		ILE				59.855	58.896	24.471		24.74			C
ATOM	1508		ILE				59.447	60.804	22.904		25.11			C
ATOM	1509		ILE				58.854	59.350	25.526		25.63			C
ATOM	1510	N			314		61.962	60.609	20.596		27.37			N
ATOM	1511	CA			314		62.451	61.673	19.729		29.50			С
ATOM	1512	С			314		63.927	61.641	19.369		31.01			С
ATOM	1513	0			314		64.422	62.554	18.706	1.00	32.03			0
MOTA	1514	N			315		64.636	60.598	19.791	1.00	31.66			N
MOTA	1515	CA			315		66.056	60.505	19.490	1.00	32.68			С
MOTA	1516	С			315		66.396	59.643	18.285	1.00	33.40			С
MOTA	1517	0			315		67.553	59.576	17.876		33.37			0
ATOM	1518	N			316		65.396	58.985	17.710	1.00	34.10			N
ATOM	1519	CA			316		65.644	58.137	16.555	1.00	35.23			C
MOTA	1520	C	GLY	Α	316		66.065	58.913	15.319	1.00	36.50			С

ATOM	1521	0	GLY	A	316	65.677	60.070	15.141	1.00	36.03		0
ATOM	1522	N	SER	A	317	66.857	58.276	14.460	1.00	37.55		N
MOTA	1523	CA			317	67.337	58.911	13.236	1.00	39.31	•	С
ATOM .	1524	C			317	66.171	59.337	12.356	1.00			С
MOTA	1525	0			317	66.295	60.251	11.543	1.00			0
MOTA	1526	CB			317	68.240	57.951	12.453	1.00			С
ATOM	1527	OG			317	67.512	56.826	11.980		38.86		0
ATOM	1528	N			318	65.040	58.663	12.522		42.85		N
MOTA	1529	CA			318	63.842	58.960	11.751	1.00	45.43		С
MOTA	1530	C			318	63.419	60.410	11.977		47.03		С
ATOM	1531	0			318	62.896	61.062	11.074	1.00			0
ATOM	1532	CB			318	62.667	58.043	12.165		45.77		С
ATOM	1533	CG1				63.127	56.586	12.239	1.00			С
ATOM	1534		ILE			61.541	58.171	11.171		46.37		С
ATOM	1535	CD1	ILE			63.984	56.265	13.459	1.00	46.06		С
HETATM	1536	N	CSO	Α	319	63.652	60.907	13.188	1.00	48.82		N
HETATM	1537	CA	CSO	A	319	63.290	62.276	13.544	1.00	51.09		C
HETATM	1538	CB	CSO	Α	319	63.435	62.481	15.053	1.00	50.48		C
METATM	1539	SG			319	62.220	61.534	16.020	1.00	49.21		S
HETATM	1540	С	CSO	A	319	64.088	63.347	12.809	1.00	52.89		С
HETATM	1541	0	CSO	А	319	 63.690	64.513	12.782	1.00	53.33		. 0
HETATM	1542	OD	CSO	Α	319	60.509	62.125	15.865	1.00	49.59		0
ATOM	1543	N	ILE	A	320	65.210	62.955	12.215	1.00	54.92		N
ATOM	1544	CA	ILE	Α	320	66.048	63.899	11.484	1.00	56.96		C
ATOM	1545	C	ILE	A	320	65.262	64.568	10.360	1.00	58.10		C
ATOM	1546	0	ILE	Α	320	65.443	65.756	10.083	1.00	58.63		0
ATOM	1547	CB	ILE	A	320	67.279	63.197	10.873	1.00	57.26		C
ATOM	1548	CG1	ILE	A	320	68.121	62.562	11.983	1.00	57.57		С
ATOM	1549	CG2	ILE	Α	320	68.113	64.201	10.089	1.00	57.46		C
ATOM	1550	CD1	ILE	Α	320	69.282	61.731	11.473	1.00	57.71		С
ATOM	1551	N	THR	Α	321	64.389	63.801	9.714	1.00	59.12		N
ATOM	1552	CA	THR	Α	321,	63.583	64.323	8.618	1.00	60.34		C
MOTA	1553	C	THR	A	321	62.103	64.387	8.985	1.00	60.84		C
ATOM	1554	0	THR	Α	321	61.257	63.773	8.330	1.00	61.34		0
MOTA	1555	CB	THR	Α	321	63.755	63.464	7.352	1.00	60.65		С
ATOM	1556	OG1	THR	Α	321	63.414	62.105	7.647	1.00	61.41		0
MOTA	1557	CG2	THR	A	321	65.195	63.524	6.860	1.00	60.98		C
MOTA	1558	N	ARG	A	322	61.806	65.138	10.040	1.00	61.12		N
ATOM .	1559	CA	ARG	Α	322	60.441	65.314	10.523	1.00	61.24		С
MOTA	1560	С	ARG	Α	322	60.445	66.385	11.606	1.00	60.69		C
ATOM ·	1561	0	ARG	Α	322	 61.501	66.723	12.145	1.00	60.84		0
MOTA	1562	CB	ARG	A.	322	59.901	63.994	11.080	1.00	62.07		С
ATOM	1563	ÇG	ARG	Α	322	58.509	64.074	11.698	1.00	63.32		C
ATOM	1564	CD	ARG	A	322	57.518	64.813	10.804	1.00	64.42		С
ATOM	1565	NE	ARG	Α	322	57.486	64.287	9.442	1.00	65.37		N
ATOM	1566	CZ	ARG	Α	322	56.737	64.792	8.466	1.00	65.78		С
ATOM	1567	NH1	ARG	А	322	55.955	65.838	8.702	1.00	65.97		N
MOTA	1568	NH2	ARG	A	322	56.774	64.258	7.253	1.00	65.94		N
ATOM	1569	N	GLU	Α	323	59.272	66.925	11.919	1.00	59.94		N
ATOM	1570	CA	GLU	Α	323	59.174	67.960	12.940	1.00	59.06		С
MOTA	1571	С	GLU	Α	323	58.885	67.393	14.325	1.00	57.87		C
MOTA	1572	0	GLU	A	323	58.236	66.355	14.466	1.00			0
ATOM	1573	CB	GLU			58.096	68.981	12.570	•	59.76		C
ATOM	1574	CG			323	57.938	70.098	13.597		60.62		C
ATOM	1575	CD			323	59.243	70.833	13.897		61.14		С
MOTA	1576	OE1	GLU			59.296	71.537	14.928		61.68		0
ATOM	1577		GLU			60.211	70.719	13.113		61.24		0

ATOM 1578 N GLN A 324 59.379 68.091 15.343 1.00 56.34 N A ATOM 1579 CA GLN A 324 59.379 68.091 15.343 1.00 56.34 N A ATOM 1580 C GLN A 324 57.726 67.648 17.141 1.00 53.18 C A ATOM 1581 O GLN A 324 57.726 67.648 17.141 1.00 53.18 C A ATOM 1582 C GLN A 324 59.956 68.634 17.658 1.00 55.79 C A ATOM 1582 C GLN A 324 61.329 68.271 17.658 1.00 55.79 C A ATOM 1583 C GLN A 324 61.329 68.271 18.094 1.00 56.75 C A ATOM 1584 C D GLN A 324 61.329 68.247 18.094 1.00 57.57 C A ATOM 1586 N B GLN A 324 61.220 66.843 18.891 1.00 57.57 C A ATOM 1586 N B GLN A 324 61.220 66.843 18.891 1.00 57.57 C A ATOM 1586 N B LYS A 325 57.357 66.607 17.880 1.00 58.36 N A ATOM 1587 C LYS A 325 57.357 66.607 17.880 1.00 59.89 N A ATOM 1589 C LYS A 325 55.992 66.607 17.880 1.00 50.98 N A ATOM 1589 C LYS A 325 55.860 67.276 19.651 1.00 46.62 C A ATOM 1590 O LYS A 325 55.860 67.276 19.651 1.00 46.62 C A ATOM 1591 C B LYS A 325 55.860 67.276 19.651 1.00 46.62 C A ATOM 1591 C B LYS A 325 55.860 67.276 19.651 1.00 46.62 C A ATOM 1591 C B LYS A 325 55.860 67.276 19.651 1.00 46.62 C A ATOM 1592 C G LYS A 325 55.860 67.276 19.651 1.00 49.79 C A ATOM 1593 C B LYS A 325 55.860 67.276 19.601 1.00 47.07 C A ATOM 1593 C B LYS A 325 55.860 67.997 18.648 1.00 49.79 C A ATOM 1593 C B LYS A 325 55.860 67.376 18.648 1.00 49.79 C A ATOM 1593 C B LYS A 325 55.860 67.376 18.648 1.00 49.79 C A ATOM 1593 C B LYS A 325 55.033 63.046 20.668 1.00 51.53 C A ATOM 1597 C B LYS A 325 55.033 63.046 20.668 1.00 51.53 C A ATOM 1599 C G LYS A 325 55.793 68.697 67.701 20.193 1.00 43.50 N A ATOM 1599 C G LYS A 326 55.973 66.697 67.701 20.193 1.00 43.50 N A ATOM 1599 C G LY A 326 55.973 66.697 67.701 20.193 1.00 43.50 N A ATOM 1599 C G LY A 326 55.973 66.697 67.701 20.193 1.00 43.50 N A ATOM 1600 N LLE A 327 57.422 66.405 22.569 1.00 36.05 N A ATOM 1600 N LLE A 327 57.866 69.39 67.701 20.193 1.00 43.50 N A ATOM 1600 C C LLE A 327 55.636 69.39 67.701 20.193 1.00 30.44 5 C A ATOM 1600 C C LLE A 327 55.636 62.390 22.89 1.00 36.05 N A ATOM 1600 C C LLE A 327 55.636 62.390 22.89 1.00 35.											
ATOM 1580 C GLN A 324 55.726 67.648 17.141 1.00 53.18 C C ATOM 1582 C G GLN A 324 55.947 68.537 16.794 1.00 53.10 C O ATOM 1583 C G GLN A 324 61.319 68.237 16.794 1.00 55.79 C C ATOM 1583 C G GLN A 324 61.329 68.127 18.094 1.00 55.75 C C ATOM 1585 C G GLN A 324 61.329 68.127 18.094 1.00 56.75 C C ATOM 1585 C R GLN A 324 61.329 66.430 18.191 1.00 57.57 C C ATOM 1585 C R GLN A 324 60.430 66.746 19.830 1.00 58.20 C C ATOM 1585 C R GLN A 324 60.430 66.746 19.830 1.00 58.20 C C ATOM 1585 C R L X A 325 57.357 66.607 17.880 1.00 58.36 N A ATOM 1587 N LX B 325 57.357 66.607 17.880 1.00 50.98 N A ATOM 1589 C L X B 325 55.992 66.461 18.367 1.00 48.78 C ATOM 1589 C L X B 325 55.992 66.461 18.367 1.00 46.62 C A ATOM 1590 C LX B 325 55.992 66.461 18.367 1.00 46.62 C ATOM 1590 C LX B 325 55.680 67.276 19.651 1.00 46.62 C ATOM 1591 C LX B 325 55.680 64.987 18.648 1.00 47.07 C ATOM 1593 C LX B 325 54.757 67.518 20.140 1.00 47.07 C ATOM 1593 C LX B 325 54.094 63.274 19.651 1.00 50.84 C ATOM 1593 C LX B 325 54.094 63.024 19.00 50.84 C ATOM 1593 C LX B 325 54.094 63.024 19.00 50.84 C ATOM 1595 C LX B 325 54.094 63.024 19.00 50.85 C ATOM 1595 C LX B 325 54.094 63.024 19.00 50.85 C ATOM 1595 C LX B 325 55.00 60.90 60.90 60.90 50.84 C ATOM 1595 C LX B 325 55.00 60.90 60.90 60.90 50.84 C ATOM 1595 C C LX B 325 55.00 60.90 60.90 60.90 50.84 C ATOM 1595 C C LX B 325 55.00 60.90 60.90 60.90 50.84 C ATOM 1595 C C LX B 325 55.00 60.90 60.90 60.90 50.84 C ATOM 1595 C C LX B 325 50.90 60.90 60.90 60.90 50.84 C ATOM 1595 C C GLY B 326 56.997 67.701 20.193 1.00 43.50 N ATOM 1595 C C GLY B 326 56.997 67.701 20.193 1.00 43.50 N ATOM 1590 C GLY B 326 56.997 67.701 20.193 1.00 43.50 N ATOM 1500 C GLY B 326 57.336 68.490 21.00 30.00 60.50 N ATOM 1600 C G LX B 327 57.836 65.993 67.900 60.40 80 60.90 6	MOTA	1578	N	${\tt GLN}$	A	324	59.379	68.091	15.343	1.00 56.34	N
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ATOM 1619 NE ARG A 329 65.626 64.149 30.692 1.00 24.50 N ATOM 1620 CZ ARG A 329 65.577 63.743 31.955 1.00 25.99 C ATOM 1621 NH1 ARG A 329 64.986 62.595 32.267 1.00 24.83 N ATOM 1622 NH2 ARG A 329 66.104 64.497 32.909 1.00 26.04 N ATOM 1623 N GLY A 330 67.054 64.458 25.304 1.00 24.47 N ATOM 1624 CA GLY A 330 68.305 63.977 24.737 1.00 24.08 C ATOM 1625 C GLY A 330 68.487 62.533 25.182 1.00 24.18 C ATOM 1626 O GLY A 330 68.857 61.655 24.254 1.00 22.92 O ATOM 1627 N GLN A 331 68.857 61.655 24.254 1.00 24.04 N ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1629 C GLN A 331 69.737 59.033 26.503 1.00 24.57 O ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C	MOTA	1617	CG .	ARG	. A	329	65.375	64.095		1.00 25.11	С
ATOM 1620 CZ ARG A 329 65.577 63.743 31.955 1.00 25.99 C ATOM 1621 NH1 ARG A 329 64.986 62.595 32.267 1.00 24.83 N ATOM 1622 NH2 ARG A 329 66.104 64.497 32.909 1.00 26.04 N ATOM 1623 N GLY A 330 67.054 64.458 25.304 1.00 24.47 N ATOM 1624 CA GLY A 330 68.305 63.977 24.737 1.00 24.08 C ATOM 1625 C GLY A 330 68.487 62.533 25.182 1.00 24.18 C ATOM 1626 O GLY A 330 68.292 62.222 26.358 1.00 22.92 O ATOM 1627 N GLN A 331 68.857 61.655 24.254 1.00 24.04 N ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1630 O GLN A 331 69.737 59.033 26.503 1.00 24.49 C ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C	ATOM	1618	CD	ARG	Α	329	65.056	63.413	29.568	1.00 24.72	C
ATOM 1621 NH1 ARG A 329 64.986 62.595 32.267 1.00 24.83 N ATOM 1622 NH2 ARG A 329 66.104 64.497 32.909 1.00 26.04 N ATOM 1623 N GLY A 330 67.054 64.458 25.304 1.00 24.47 N ATOM 1624 CA GLY A 330 68.305 63.977 24.737 1.00 24.08 C ATOM 1625 C GLY A 330 68.487 62.533 25.182 1.00 24.18 C ATOM 1626 O GLY A 330 68.292 62.222 26.358 1.00 22.92 O ATOM 1627 N GLN A 331 68.857 61.655 24.254 1.00 24.04 N ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1629 C GLN A 331 70.004 59.909 25.679 1.00 24.49 C ATOM 1630 O GLN A 331 69.415 59.470 23.286 1.00 24.17 C ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.47 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33	MOTA	1619	NE	ARG	A	329	65.626	64.149	30.692	1.00 24.50	N
ATOM 1622 NH2 ARG A 329 66.104 64.497 32.909 1.00 26.04 N ATOM 1623 N GLY A 330 67.054 64.458 25.304 1.00 24.47 N ATOM 1624 CA GLY A 330 68.305 63.977 24.737 1.00 24.08 C ATOM 1625 C GLY A 330 68.487 62.533 25.182 1.00 24.18 C ATOM 1626 O GLY A 330 68.292 62.222 26.358 1.00 22.92 O ATOM 1627 N GLN A 331 68.857 61.655 24.254 1.00 24.04 N ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1629 C GLN A 331 70.004 59.909 25.679 1.00 24.49 C ATOM 1630 O GLN A 331 69.415 59.470 23.286 1.00 24.17 C ATOM 1631 CB GLN A 331 69.415 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C	MOTA	1620	CZ	ARG	A	329	65.577	63.743	31.955	1.00 25.99	C
ATOM 1623 N GLY A 330 67.054 64.458 25.304 1.00 24.47 N ATOM 1624 CA GLY A 330 68.305 63.977 24.737 1.00 24.08 C ATOM 1625 C GLY A 330 68.487 62.533 25.182 1.00 24.18 C ATOM 1626 O GLY A 330 68.292 62.222 26.358 1.00 22.92 O ATOM 1627 N GLN A 331 68.857 61.655 24.254 1.00 24.04 N ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1629 C GLN A 331 70.004 59.909 25.679 1.00 24.49 C ATOM 1630 O GLN A 331 69.737 59.033 26.503 1.00 24.57 O ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C	ATOM	1621	NH1	ARG	А	329	64.986	62.595		1.00 24.83	N
ATOM 1624 CA GLY A 330 68.305 63.977 24.737 1.00 24.08 C ATOM 1625 C GLY A 330 68.487 62.533 25.182 1.00 24.18 C ATOM 1626 O GLY A 330 68.292 62.222 26.358 1.00 22.92 O ATOM 1627 N GLN A 331 68.857 61.655 24.254 1.00 24.04 N ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1629 C GLN A 331 70.004 59.909 25.679 1.00 24.49 C ATOM 1630 O GLN A 331 69.737 59.033 26.503 1.00 24.57 O ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C	MOTA	1622	NH2	ARG	Α	329	66.104	64.497	32.909	1.00 26.04	N
ATOM 1625 C GLY A 330 68.487 62.533 25.182 1.00 24.18 C ATOM 1626 O GLY A 330 68.292 62.222 26.358 1.00 22.92 O ATOM 1627 N GLN A 331 68.857 61.655 24.254 1.00 24.04 N ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1629 C GLN A 331 70.004 59.909 25.679 1.00 24.49 C ATOM 1630 O GLN A 331 69.737 59.033 26.503 1.00 24.57 O ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C	MOTA	1623	N				67.054	64.458	25.304	1.00 24.47	N
ATOM 1626 O GLY A 330 68.292 62.222 26.358 1.00 22.92 O ATOM 1627 N GLN A 331 69.022 60.230 24.551 1.00 24.04 N ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1629 C GLN A 331 70.004 59.909 25.679 1.00 24.49 C ATOM 1630 O GLN A 331 69.737 59.033 26.503 1.00 24.57 O ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C			CA				68.305	63.977	24.737	1.00 24.08	
ATOM 1627 N GLN A 331 68.857 61.655 24.254 1.00 24.04 N ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1629 C GLN A 331 70.004 59.909 25.679 1.00 24.49 C ATOM 1630 O GLN A 331 69.737 59.033 26.503 1.00 24.57 O ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C	MOTA		C				68.487	62.533	25.182	1.00 24.18	C
ATOM 1628 CA GLN A 331 69.022 60.230 24.551 1.00 24.22 C ATOM 1629 C GLN A 331 70.004 59.909 25.679 1.00 24.49 C ATOM 1630 O GLN A 331 69.737 59.033 26.503 1.00 24.57 O ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C			0				68.292			1.00 22.92	0
ATOM 1629 C GLN A 331 70.004 59.909 25.679 1.00 24.49 C ATOM 1630 O GLN A 331 69.737 59.033 26.503 1.00 24.57 O ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C											
ATOM 1630 O GLN A 331 69.737 59.033 26.503 1.00 24.57 O ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C						••					
ATOM 1631 CB GLN A 331 69.445 59.470 23.286 1.00 24.17 C ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C	1										
ATOM 1632 CG GLN A 331 69.411 57.946 23.436 1.00 24.47 C ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C											
ATOM 1633 CD GLN A 331 67.988 57.392 23.540 1.00 25.33 C											
ATOM 1634 OE1 GLN A 331 67.777 56.262 23.989 1.00 25.75 O											
	ATOM	1634	OE1	GLN	Α	331	67.777	56.262	23.989	1.00 25.75	0

MOTA	1635	NE2	GLN	A	331	67.013	58.183	23.112	1.00 24			N
ATOM	1636	N	ALA	Α	332	71.139	60.602	25.713	1.00 23	3.98		N
ATOM	1637	CA	ALA	Α	332	72.138	60.355	26.746	1.00 23	3.64		С
MOTA	1638	C	ALA	Α	332	71.576	60.692	28.124	1.00 23			С
MOTA	1639	0	ALA	Α	332	71.673	59.892	29.058	1.00 22			0
MOTA	1640	CB	ALA	A	332	73.403	61.176	26.470	1.00 23			С
ATOM	1641	N	THR	А	333	70.982	61.875	28.245	1.00 23			N
MOTA	1642	CA	THR			70.401	62.302	29.510	1.00 23			C
ATOM	1643	C	THR			69.294	61.345	29.954	1.00 23			С
ATOM	1644	0	THR			69.163	61.040	31.144	1.00 22			0
ATOM	1645	CB	THR			69.814	63.717	29.398	1.00 23			С
MOTA	1646	OG1	THR			70.838	64.619	28.960	1.00 25			0
MOTA	1647	CG2	THR			69.273	64.179	30.749	1.00 24			С
MOTA	1648	N	ALA			68.497	60.884	28.995	1.00 22			N
MOTA	1649	CA	ALA			67.407	59.959	29.292	1.00 23			C
MOTA	1650	C	ALA			67.949	58.654	29.886	1.00 22			C
MOTA	1651	0	ALA			67.456	58.175	30.907	1.00 22			0
MOTA	1652	CB	ALA			66.602	59.671	28.020	1.00 22			C
MOTA	1653	N	VAL			68.965	58.085	29.251	1.00 22		٠	N
MOTA	1654	CA	VAL			69.556	56.840	29.737	1.00 21			С
MOTA	1655	C	VAL	Α	335	70.150	57.026	31.134	1.00 22			\mathbf{C}_{\cdot}
MOTA	1656	0	VAL	Α	335	69.869	56.249	32.047	1.00 22			0
MOTA	1657	CB	VAL			70.656	56.334	28.765	1.00 23			С
MOTA	1658	CG1	VAL	A	335	71.411	55.152	29.378	1.00 22			С
ATOM	1659	CG2	VAL	Α	335	70.015	55.917	27.440	1.00 22			С
MOTA	1660	N	ILE	Α	336 _.	70.952	58.071	31.302	1.00 22			N
MOTA	1661	CA	ILE	Α	336	71.588	58.352	32.583	1.00 23			С
MOTA	1662	С	ILE	Α	336	70.569	58.499	33.710	1.00 23		*	С
MOTA	1663	0 -	ILE	A	336	70.751	57.941	34.796	1.00 23			0
MOTA	1664	CB	ILE	Α	336	72.437	59.636	32.498	1.00 23			С
MOTA	1665	CG1	ILE	А	336	73.614	59.406	31.545	1.00 23			С
MOTA	1666	CG2	ILE	Α	336	72.929	60.044	33.888	1.00 23			С
ATOM	1667	CD1	ILE	Α	336	74.395	60.668	31.215	1.00 23			C
MOTA	1668	N	ASP	А	337	69.500	59.248	33.449	1.00 24			N
ATOM	1669	CA			337	68.457	59.471	34.447	1.00 2			C
ATOM	1670	С			337	67.713	58.179	34.777	1.00 2			C
MOTA	1671	0			337	67.506	57.849	35.947	1.00 2			0
MOTA	1672	CB			337	67.446	60.505	33.948	1.00 2			С
MOTA	1673	CG			-337	66.441	60.891		1.00 2			C
MOTA	1674		ASP				61.195		1.00 2			0
MOTA	1675	OD2	ASP			66.821	60.902	36202	1.00 2			0
MOTA	1676	N			338	67.293	57.455	33.743	1.00 2			N
MOTA	1677	CA			338	66.569	56.206	33.953	1.00 2			C
MOTA	1678	C			338	67.430	55.171	34.672	1.00 2			C
MOTA	1679	0			338	66.948	54.471	35.557	1.00 2			0
MOTA	1680	CB			338	66.075	55.611	32.615	1.00 2			C
MOTA	1681		VAL			65.518	54.204	32.839	1.00 2			C
MOTA	1682	CG2	VAL			64.985	56.514	32.023	1.00 2			C
MOTA	1683	N			339	68.700	55.078	34.284	1.00 2			N
MOTA	1684	CA			339	69.622	54.129	34.903	1.00 2			C
MOTA	1685	C			339	69.776	54.432	36.398	1.00 2			C
MOTA	1686	0			339	69.853	53.520	37.219	1.00 2			0
MOTA	1687	CB			339		. 54.174	34.214	1.00 2			C
MOTA	1688		VAL			72.079	53.494	35.099				C
MOTA	1689		VAL			70.936	53.465	32.855	1.00 2			C
MOTA	1690	N			340	69.821	55.712	36.749	1.00 2			N
MOTA	1691	CA	ALA	A	340	69.957	56.085	38.155	1.00 2	3.22		С

MOTA	1692	С	ALA	Α	340	68.717	55.623	38.928		22.99		С
ATOM	1693	0	ALA	А	340	68.818	55.112	40.048		23.73		0
MOTA	1694	CB	ALA	Α	340	70.140	57.599	38.283		23.33		С
MOTA	1695	N	GLU	Α	341	67.549	55.788	38.320		22.81		N
ATOM`	1696 ·	CA	GLU	Α	341	66.298	55.376	38.955		23.25		C
MOTA	1697	С	GLU	А	341	66.234	53.851	39.047	1.00	22.89		C
ATOM	1698	0	GLU	A	341	65.740	53.296	40.029	1.00	22.02		0
ATOM	1699	CB	GLU	А	341	65.103	55.885	38.146	1.00	23.80		C
MOTA	1700	CG	GLU	Α	341	63.786	55.897	38.910	1.00	26.95		C
ATOM	1701	CD	GLU	A	341	63.827	56.810	40.130	1.00	29.07		C
MOTA	1702	OE1	GLU	Α	341	64.433	57.902	40.052	1.00	30.17		0
MOTA	1703	OE2	GLU	Α	341	63.240	56.441	41.165	1.00	30.84		0
ATOM	1704	N	ARG	А	342	66.736	53.179	38.014		22.30		N
MOTA	1705	CA	ARG	Α	342	66.737	51.722	37.979	1.00	22.47		C
MOTA	1706	С	ARG	Α	342	67.639	51.169	39.084	1.00	22.30		C
ATOM	1707	0	ARG	А	342	67.303	50.182	39.732	1.00	22.02		0
MOTA	1708	CB	ARG	Α	342	67.205	51.233	36.598	1.00	22.21		C
MOTA	1709	CG	ARG	Α	342	67.165	49.717	36.393	1.00	21.30		C
ATOM	1710	CD	ARG	Α	342	68.428	49.027	36.910	1.00	21.14		C
ATOM	1711	NE	ARG			69.657	49.497	36.266	1.00	21.04		N
MOTA	1712	CZ	ARG			70.024	49.221	35.012	1.00	21.58		C
ATOM	1713		ARG			69.260	48.468	34.227	1.00	20.91		N
MOTA	1714	NH2	ARG	Α	342	71.175	49.686	34.543	1.00	21.45		N
MOTA	1715	Ŋ	ASN	Α	343	68.780	51.813	39.304	1.00	22.59		N
ATOM	1716	CA	ASN			69.697	51.356	40.343	1.00	23.77		С
ATOM	1717	С	ASN			69.096	51.613	41.721	1.00	24.38		C
MOTA	1718	0	ASN			69.274	50.816	42.643	1.00	23.51		0
MOTA	1719	CB			343	71.060	52.046	40.201	1.00	23.94		C
ATOM	1720	CG			343	71.798	51.608	38.948	1.00	24.43		C
ATOM	1721		ASN			71.500	50.554	38.386	1.00	24.77		0
ATOM	1722		ASN			72.775	52.404	38.513	1.00	24.50		N
ATOM	1723	N			344	68.368	52.718	41.849	1.00	24.94		N
ATOM	1724	CA			344	67.717	53.063	43.104	1.00	26.62		C
ATOM	1725	С			344	66.626	52.029	43.368	1.00	26.38		C
ATOM	1726	0			344	66.461	51.551	44.492	1.00	26.78		0
ATOM	1727	CB			344	67.106	54.465	43.008	1.00	29.24		C
ATOM	1728	CG			344	66.398	54.943	44.267	1.00	32.28		C
ATOM	1729	CD			344	65.866	56.358	44.078	1.00	34.61		C
ATOM		CE			344	 65.196	56.878	45.343	1.00	36.69		C
ATOM	1731	NZ			344	66.161	57.002	46.475	1.00	38.80		N
MOTA	1732	N.			345	65.888	51.681	42.318	1.00	25.59		N
MOTA	1733	CA			345	64.811	50.702	42.412	1.00	25.49		C
MOTA	1734	С			345	65.366	49.339	42.841	1.00	25.79		С
ATOM	1735	0			345	64.746	48.627	43.635	1.00	24.45		0
MOTA	1736	CB			345	64.117	50.566	41.057	1.00	25.37		C
MOTA	1737	CG			345	62.815	49.801	41.089	1.00	25.96		C
ATOM	1738	CD1	TYR			61.626	50.427	41.460	1.00	26.32		C
MOTA	1739		TYR			62.764	48.459	40.713	1.00	26.30		С
MOTA	1740		TYR			60.415	49.738	41.446	1.00	27.08		C
MOTA	1741		TYR			61.558	47.759	40.697	1.00	27.11		C
ATOM	1742	CZ			345	60.391	48.406	41.061	1.00	27.19		C
MOTA	1743	ОН			345	 59.195	47.735	41.008	1.00	28.86		0
ATOM	1744	N			346	66.530	48.983	42.305	1.00	26.33		N
ATOM	1745	CA			346	67.181	47.713	42.632		27.73		C
ATOM	1746	C			346	67.537	47.684	44.118		28.91		С
ATOM	1747	0			346	67.337		44.798	1.00	28.66		O,
ATOM	1748	CB			346	68.450	47.540	41.793	1.00	27.70		С
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MOTA	1749	CG	PHE	A٠	346	69.269	46.331	42.163	1.00	27.99		C
ATOM	1750	CD1	PHE	Α	346	68.773	45.047	41.959	1.00	27.87		C
ATOM	1751	CD2	PHE	Α	346	70.536	46.480	42.723	1.00	28.85		С
MOTA	1752	CE1	PHE	Α	346	69.526	43.923	42.304	1.00	27.89		C
MOTA	1753	CE2	PHE	Α	346	71.303	45.361	43.076	1.00	29.71		C
MOTA	1754	CZ	PHE	Α	346	70.793	44.080	42.864	1.00	29.06		C
MOTA	1755	N	GLU	Α	347	68.059	48.798	44.616	1.00	30.12		N
ATOM	1756	CA	GLU			68.430	48.897	46.021	1.00	32.28		C
ATOM	1757	С	GLU			67.227	48.820	46.958	1.00	31.98		C
ATOM	1758	0	GLU			67.329	48.280	48.056	1.00	31.99		0
ATOM	1759	CB	GLU			69.189	50.200	46.280	1.00	33.95	•	С
ATOM	1760	CG	GLU			70.645	50.150	45.853	1.00	38.56		С
ATOM	1761	CD	GLU			71.454	51.319	46.386	1.00	41.08		С
ATOM	1762	OE1				71.294	51.673	47.576		42.98		0
ATOM	1763		GLU			72.265	51.875	45.619		43.56		0
ATOM	1764	N	GLU			66.091	49.352	46.522		31.64		N
ATOM	1765	CA	GLU			64.888	49.347	47.348		31.87		С
ATOM	1766	C	GLU	-		64.124	48.031	47.330		30.98		С
ATOM	1767	0	GLU			63.576	47.617	48.350		31.10		0
ATOM	1768	CB	GLU			63.911	50.439	46.897		33.10		C
ATOM	1769	CG	GLU			64.506	51.812	46.664		35.32		Ċ
ATOM	1770	CD	GLU			63.494	52.779	46.059		36.44		Ċ
ATOM	1771		GLU			62.716	52.775	45.178		37.22		ō
ATOM	1772		GLU			63.481	53.961	46.454		38.05		Ö
ATOM	1772	N			349	64.079	47.381	46.171		29.37		N
	1774	CA			349	63.316	46.147	46.016		28.42		C
ATOM						64.107	44.864	45.790		28.26		C
ATOM	1775	C			349 349	63.563	43.775	45.730		28.54		0
ATOM	1776	0						44.829		28.53		C
ATOM	1777	CB			349	62.347	46.267	43.611		26.68		0
ATOM	1778	OG1	THR			63.106	46.331 47.525	44.956		27.99		C
ATOM	1779		THR			61.489	44.982	45.423		27.91		N
ATOM	1780	N			350	65.375	44.982	45.423		27.45		C
ATOM	1781	CA			350	66.153				26.56		C
ATOM	1782	C			350	65.860	43.276	43.743		27.60	,	0
ATOM	1783	0			350 .	66.367	42.235	43.339		25.92		N
ATOM	1784	N			351	65.034	44.005	42.995		24.44		C
ATOM	1785	CA			351	64.687	43.614	41.625		23.82		C
ATOM	1786	C			351	65.530	44.395	40.619		22.61		0
ATOM	1787	0			351	65.557	45.627	40.649		25.48		C
MOTA	1788	CB			351		43.913			25.40		C
ATOM	1789		ILE			62.281	43.222	42.310		25.21		C
ATOM	1790		ILE			62.880	43.449	39.873		26.39		C
ATOM	1791		ILE			60.810	43.615	42.169				N
ATOM	1792	N			352		43.683	39.728		23.12		
MOTA	1793	CA			352	67.024	44.339	38.708		22.28		C
ATOM	1794	С			352	66.274	44.290	37.389		22.46		
MOTA	1795	0.			352	66.033	43.210	36.845		21.68		0
ATOM	1796	CB			352	68.375	43.647	38.518		22.40		C
ATOM	1797	CG			352	69.269	44.375	37.526		22.27		C
ATOM	1798		TYR			70.058	45.451	37.932		22.07		C
ATOM	1799		TYR			69.296	44.012	36.176		22.89		С
MOTA	1800		TYR			70.852	46.151	37.028		22.81		C
ATOM	1801		TYR			70.094	44.714	35.252		22.60		C
MOTA	1802	CZ			352	70.868	45.779	35.691		22.45		C
MOTA	1803	OH			352	71.676	46.468	34.814		22.10		0
MOTA	1804	Ņ			353	65.912	45.462	36.876		22.15		N
MOTA	1805	CA	ILE	A	353	65.196	45.556	35.610	1.00	22.13		С

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MOTA	1806	С	ILE	A	353	66.119	46.052	34.495		21.86		С
ATOM.	1807	0	ILE	Α	353	66.603	47.188	34.531	1.00	21.86		0
MOTA	1808	CB	ILE	Α	353	63.996	46.523	35.721	1.00	23.05		С
ATOM	1809	CG1	ILE	Α	353	63.036	46.030	36.817	1.00	23.41		С
ATOM	1810		ILE			63.278	46.614	34.374	1.00	21.86		С
ATOM	1811	CD1	ILE			61.863	46.936	37.063		24.85		С
ATOM	1812	N	PRO			66.388	45.201	33.495		21.74		N
						67.263	45.626	32.397		21.25		C
ATOM	1813	CA	PRO									C
ATOM	1814	C	PRO			66.608	46.780	31.649		21.17		0
ATOM	1815	0	PRO			65.385	46.825	31.534		21.72		
MOTA		CB	PRO			67.360	44.373	31.524		21.72		C
MOTA	1817	CG	PRO			67.181	43.240	32.529		20.93		С
MOTA	1818	CD	PRO			66.051	43.769	33.382		21.57		C
ATOM	1819	N	VAL	Α	355	67.406	47.722	31.159	1.00	20.15		N
ATOM	1820	CA	VAL	Α	355	66.841	48.829	30.396	1.00	19.73		C
MOTA	1821	C	VAL	A	355	67.482	48.842	29.022	1.00	19.50		С
ATOM	1822	0	VAL	A	355	68.629	48.430	28.851	1.00	19.88		ο`
ATOM	1823	СВ	VAL			67.032	50.206	31.094	1.00	18.66		С
MOTA	1824		VAL			66.254	50.226	32.394		18.46		С
ATOM	1825		VAL			68.514	50.497	31.333		18.65		C
ATOM			CYS			66.723	49.312	28.043		19.68		N
	1826	N										C
ATOM	1827	CA			356"	67.185	49.346	26.666		20.26		
ATOM	1828	C	CYS			67.273	50.761	26.110		20.70		C
ATOM	1829	0	CYS			66.297	51.509	26.161		20.96		0
ATOM	1830	CB	CYS			66.228	48.522	25.796		20.28		С
ATOM	1831	SG	CYS	Α	356	66.486	48.701	24.007		22.73		S
MOTA	1832	N	SER	Α	357	68.440	51.129	25.586	1.00	20.27		N
ATOM	1833	CA	SER	Α	357	68.597	52.447	24.981	1.00	20.16		С
ATOM	1834	C	SER	A	357	68.088	52.277	23.553	1.00	20.30		С
ATOM	1835	0	SER	Α	357	68.713	51.599	22.734	1.00	19.54		0
ATOM	1836	CB			357	70.061	52.882	24.962		20.20		С
ATOM	1837	OG	SER			70.163	54.193	24.432		20.16		0
ATOM	1838	N	ASP			66.951	52.899	23.262		20.12		N
ATOM	1839	CA	ASP			66.327	52.767	21.955		21.37		C
							54.009	21.070		21.92		C
ATOM	1840	C	ASP			66.441				.22.18		0
ATOM	1841	0			358	65.862	55.057	21.367				
ATOM	1842	CB			358	64.855	52.370	22.166		20.81		C
ATOM	1843	CG	ASP			64.081	52.214	20.867		22.08		C
ATOM	1844		ASP			64.703	52.059	19.791		21.34	•	0
ATOM	1845	OD2	ASP	A	358	62.834	52.229	20.937		20.69		0
ATOM	1846	N ·	GLY	А	359	67.204	53.875	19.986	1.00	22.92		N
MOTA	1847	CA	GLY	Α	359	67.381	54.964	19.040	1.00	23.74		С
ATOM	1848	C	GLY	A	359	68.538	55.905	19.328	1.00	25.08		С
ATOM	1849	0	GLY	А	359	69.078	55.928	20.431	1.00	24.78		0
ATOM	1850	N			360	68.932	56.678	18.323	1.00	25.97		N
ATOM	1851	CA			360	70.007	57.633	18.517	1.00	27.86		C
ATOM	1852	С			360	71.419	57.132			28.88		С
ATOM	1853	0			360	72.367	57.904	18.417		29.93		0
ATOM	1854	N			361	71.581	55.855	17.961		29.68		N
							55.329	17.706		30.57		C
ATOM	1855	CA			361	72.918						С
ATOM	1856	C			361	73.309	55.719	16.282		31.81		
MOTA	1857	0			361	72.765	55.196	15.310		31.75		0
MOTA	1858	CB			361	72.971	53.789	17.838		30.18		С
MOTA	1859		ILE			72.603	53.368	19.266		29.88		С
MOTA	1860	CG2	ILE	Α	361	74.366	53.282	17.481	1.00	30.01		C
MOTA	1861	CD1	ILE	Α	361	73.605	53.792	20.328	1.00	28.84		С
ATOM	1862	N	VAL	Α	362	74.249	56.648	16.167	1.00	32.99		N

ATOM	1863	CA	VAL	A	362	74.699	57.110	14.862	1.00	33.95		C
MOTA	1864	C	VAL	A	362	76.028	56.463	14.483	1.00	34.24		С
MOTA	1865	0	VAL	Α	362	76.203	56.015	13.351	1.00	35.04		0
MOTA	1866	CB	VAL	A	362	74.851	58.646	14.854	1.00	34.42		C
MOTA	1867	CG1	VAL	Α	362	75.233	59.131	13.462	1.00	34.82		C
ATOM	1868	CG2	VAL	A	362	73.555	59.292	15.304	1.00	34.82		C
MOTA	1869	N	TYR			76.953	56.404	15.438	1.00	33.91		N
ATOM	1870	CA	TYR	Ά	363	78.271	55.813	15.210	1.00	33.19		C
ATOM	1871	C	TYR	Α	.363	78.507	54.649	16.163		31.86		С
MOTA	1872	0	TYR			77.862	54.561	17.207		31.05		0
MOTA	1873	CB	TYR			79.350	56.877	15.411		34.45		С
MOTA	1874	CG	TYR			79.142	58.094	14.544		36.04		С
ATOM	1875	CD1	TYR			79.242	58.008	13.154		37.00	*	С
MOTA	1876	CD2	TYR			78.796	59.323	15.105		36.77		C
ATOM	1877	CE1	TYR			78.998	59.114	12.344		38.19		C
ATOM	1878	CE2	TYR			78.548	60.435	14.304		37.90		С
ATOM	1879	CZ	TYR			78.649	60.323	12.926		38.55		C
ATOM	1880	OH	TYR			78.390	61.415	12.130		40.47		0
ATOM	1881	N	ASP			79.432	53.760	15.813		30.55		N
ATOM	1882	CA	ASP			79.717	52.610	16.668		29.67	-	C
ATOM	1883	C	ASP			80.055	52.987	18.108		28.54		C
ATOM	1884	0	ASP			79.621	52.316	19.043		28.30		0
ATOM	1885	CB	ASP			80.871	51.772	16.109		30.75		C
ATOM	1886	CG	ASP			80.511	51.052	14.819		31.62		C
ATOM	1887		ASP			79.346	50.634	14.647		31.07		0
ATOM	1888		ASP			81.413	50.887	13.981		33.54		0
ATOM ATOM	1889 1890	N CA	TYR			80.828	54.054	18.293		26.82		N
ATOM			TYR			81.214	54.449	19.642		26.01		C
ATOM	1891 1892	C 0	TYR TYR			80.021	54.874 54.925	20.499		25.10		
ATOM	1893	CB	TYR			80.117 82.295	55.541	21.723 19.588		24.73 25.94		O C
ATOM	1894	CG	TYR			81.804	56.962	19.451		26.33		, C
ATOM	1895	CD1	TYR			81.582	57.751	20.578		25.79		C
ATOM	1896	CD2	TYR			81.624	57.542	18.193		26.48		C
ATOM	1897	CE1	TYR			81.203	59.086	20.459		27.08		C
ATOM	1898	CE2	TYR			81.242	58.876	18.063		27.27		C
ATOM	1899	CZ	TYR			81.036	59.640	19.198		27.74		C
ATOM	1900	OH	TYR			80.675	60.962	19.074		29.07		Ö
MOTA	1901	N	HIS			78.892	55.164	19.858		24.53		N
MOTA	1902	CA	HIS			77.685	55.534	20.591		24.28		. C
ATOM	1903	C.	HIS			77.190	54.300	21.339		23.77		C
MOTA	1904	0	HIS			76.569	54.411	22.399		23.59		0
MOTA	1905	CB	HIS			76.589	56.017	19.641		24.35		С
MOTA	1906	CG	HIS	Α	366	76.799	57.409	19.134	1.00	25.11		С
MOTA	1907	ND1	HIS	Α	366	77.870	58.187	19.517	1.00	25.78		N
MOTA	1908	CD2	HIS	А	366	76.059	58.173	18.295	1.00	25.31		C
MOTA	1909	CE1	HIS	A	366	77.779	59.372	18.938	1.00	25.96		С
ATOM	1910	NE2	HIS	A	366	76.690	59.389	18.191	1.00	25.85		N
MOTA	1911	N	MET	Α	367	77.463	53.129	20.773	1.00	23.23		N
MOTA	1912	CA.	MET	Α	367	77.062	51.863	21.388	1.00	23.44		C
MOTA	1913	C	MET			77.785	51.715	22.721		22.42		C
MOTA	1914	0	MET			77.180	51.385	23.735		21.74	•	0
MOTA	1915	CB	MET			77.437	50.672	20.494		23.55		C
MOTA	1916	CG	MET			76.680	50.582	19.169		25.18		С
ATOM	1917	SD	MET			77.253	49.158	18.204		26.50		S
MOTA	1918	CE	MET			76.270	49.323	16.707		25.76		С
ATOM	1919	N	THR	A	368	79.093	51.941	22.698	1.00	22.22		N

MOTA	1920	CA	THR	А	368	79.915	51.835	23.898	1.00 22.15			С
MOTA	1921	C	THR	Α	368	79.445	52.838	24.952	1.00 21.97			C
ATOM	1922	0	THR	A	368	79.380	52.517	26.137	1.00 22.10			0
MOTA	1923	CB	THR	Α	368	81.392	52.097	23.560	1.00 22.55			С
MOTA	1924	OG1	THR	Α	368	81.735	51.369	22.373	1.00 22.22			0
ATOM	1925	CG2	THR	A	368	82.294	51.645	24.702	1.00 21.82			С
ATOM	1926	N	LEU	Α	369	79.117	54.052	24.517	1.00 21.48			N
MOTA	1927	CA	LEU	Α	369	78.640	55.087	25.431	1.00 21.65			C
ATOM	1928	С	LEU	А	369	77.318	54.693	26.096	1.00 21.14			С
MOTA	1929	0	LEU	Α	369	77.163	54.833	27.306	1.00 20.89		•	0
MOTA	1930	CB	LEU	Α	369	78.446	56.416	24.689	1.00 22.45			С
ATOM	1931	CG	LEU	А	369	79.697	57.209	24.300	1.00 24.02			С
MOTA	1932	CD1	LEU	Α	369	79.301	58.381	23.400	1.00 23.76			C
MOTA	1933	CD2	LEU	Α	369	80.397	57.710	25.567	1.00 23.98			С
ATOM	1934	N	ALA	Α	370	76.371	54.211	25.296	1.00 20.39			N
MOTA	1935	CA	ALA	Α	370	75.065	53.806	25.810	1.00 20.84			C
MOTA	1936	С	ALA	Α	370	75.242	52.732	26.877	1.00 20.22			С
ATOM	1937	0	ALA	Α	370	74.635	52.793	27.945	1.00 20.03			0
MOTA	1938	CB	ALA	Α	370	74.194	53.279	24.675	1.00 20.37	:		С
MOTA	1939	N	LEU	Α	371	76.078	51.748	26.576	1.00 20.36			N
ATOM	1940	CA	LEU	Α	371	76.343	50.669	27.516	1.00 20.12			C
MOTA	1941	·C	LEU	Α	371	77.032	51.209	28.773	1.00 20.41			С
MOTA	1942	0	LEU	Α	371	76.656	50.853	29.887	1.00 19.69			0
MOTA	1943	CB	LEU	A	371	77.222	49.602	26.854	1.00 19.81			C
MOTA	1944	CG	LEU	Α	371	76.580	48.882	25.656	1.00 20.61			C
MOTA	1945	CD1	LEU	Α	371	77.592	47.954	24.999	1.00 21.12			С
MOTA	1946	CD2	LEU	Α	371	75.364	48.092	26.127	1.00 20.77			С
MOTA	1947	N	ALA	Α	372	78.036	52.064	28.588	1.00 20.08			N
MOTA	1948	CA	ALA	Α	372	78.772	52.640	29.712	1.00 20.58			С
MOTA	1949	C			372	77.868	53.444	30.641	1.00 21.51			C
MOTA	1950	0			372	78.064	53.450	31.858	1.00 21.21			0
MOTA	1951	CB	ALA	A	372	79.909	53.525	29.199	1.00 20.25			С
MOTA	1952	N	MET	A	373	76.883	54.126	30.065	1.00 21.00			N
MOTA	1953	CA	MET			75.947	54.923	30.852	1.00 21.56			C
MOTA	1954	C	MET	Α	373	74.960	54.065	31.641	1.00 21.75			C
MOTA	1955	0	MET	Α	373	74.187	54.588	32.449	1.00 21.78			0
MOTA	1956	CB	MET	Α	373	75.192	55.892	29.944	1.00 21.91			C
ATOM	1957	CG	MET	Α	373	76.082	56.987	29.370	1.00 22.56			C
MOTA	1958	SD	MET	Α	373	. 75.243	57.985	28.132	1.00 24.61			s
ATOM	1959	CE	MET	Α	373	76.595	59.086	27.591	1.00 23.75			C
ATOM	1960	N	GLY	Α	374	74.970	52.754	31.405	1.00 21.29			N
MOTA	1961	CA	GLY	Α	374	74.078	51.884	32.157	1.00 20.54			C
MOTA	1962	C	GLY	Α	374	73.062	51.058	31.390	1.00 20.55			C
ATOM	1963	0	GLY	Α	374 ·	72.444	50.164	31.961	1.00 20.60			0
MOTA	1964	N	ALA	A	375	72.864	51.345	30.108	1.00 20.21			N
MOTA	1965	CA	ALA	Α	375	71.910	50.562	29.332	1.00 20.36			C
ATOM	1966	C	ALA	Α	375	72.448	49.140	29.228	1.00 20.12			C
MOTA	1967	0	ALA	Α	375	73.644	48.943	29.011	1.00 19.79			0
MOTA	1968	CB	ALA	Α	375	71.731	51.166	27.932	1.00 20.49			С
ATOM	1969	N	ASP	A	376	71.573	48.151	29.399	1.00 20.05			N
MOTA	1970	CA	ASP	Α	376	71.976	46.744	29.308	1.00 20.54			С
MOTA	1971	C	ASP	Α	376	72.074	46.303	27.854	1.00 20.62			С
MOTA	1972	0	ASP	A	376	72.933	45.498	27.491	1.00 20.67			0
MOTA	1973	CB	ASP	Α	376	70.978	45.874	30.069	1.00 20.75			С
MOTA	1974	CG	ASP	Α	376	70.900	46.253	31.530	1.00 21.21			C
MOTA	1975	OD1	ASP	A	376	71.732	45.757	32.319	1.00 21.97			0
MOTA	1976	OD2	ASP	A	376	70.027	47.073	31.882	1.00 21.23			0

ATOM	1977	N	PHE	A	377	71.173	46.813	27.022	1.00	21.26	N
MOTA	1978	CA	PHE	A	377	71.220	46.501	25.604	1.00	21.16	С
MOTA	1979	C ·	PHE	Α	377	70.726	47.683	24.788	1.00	21.44	C
MOTA	1980	0	PHE	Α	377	70.186	48.647	25.336	1.00	21.24	0
MOTA	1981	CB	PHE	A	377	70.467	45.204	25.252	1.00	21.17	C
MOTA	1982	CG	PHE	А	377	69.056	45.135	25.758	1.00	22.60	C
MOTA	1983	CD1	PHE	A	377	68.791	44.771	27.077	1.00	23.03	, C
ATOM	1984		PHE			67.987	45.371	24.900	1.00	21.57	C
MOTA	1985		PHE			67.478	44.638	27.531		22.95	C
MOTA	1986	CE2	PHE			66.669	45.240	25.345		22.51	C
MOTA	1987	CZ	PHE			66.416	44.872	26.663		22.95	C
MOTA	1988	N	ILE			70.931	47.600	23.480		20.98	N
MOTA	1989	CA	ILE			70.607	48.683	22.567		21.02	C
MOTA	1990	С	ILE			69.669	48.272	21.439		20.93	C
ATOM	1991	0	ILE			69.847	47.222	20.833		20.57	0
ATOM	1992	CB	ILE			71.923	49.220	21.936		21.28	C
ATOM	1993		ILE			72.914	49.588	23.046		21.93	C
ATOM	1994	CG2	ILE			71.643	50.439	21.056		21.62	C
ATOM	1995	CD1	ILE			74.341	49.772	22.558		22.57	C
ATOM	1996	N	MÉT			68.669	49.105	21.166		20.84	N
ATOM	1997	CA	MET			67.743	48.831	20.073		21.55	C
ATOM	1998	C	MET			68.084	49.794	18.941		21.65	C
ATOM	1999	0	MET			68.230	50.998	19.164		21.66	0
ATOM	2000	CB	MET			66.284	49.028	20.503		21.25	C - C
ATOM	2001	CG	MET MET			65.303	48.766	19.356		21.22	s
ATOM	2002	SD				63.576	48.745	19.833		22.14	C
ATOM ATOM	2003 2004	CE N	MET			63.437 68.226	47.038 49.262	20.433 17.731		22.39	N
ATOM	2004	CA	LEU			68.575	50.092	16.584		22.48	C
ATOM	2005	C	LEU			67.703	49.788	15.373		22.97	C
ATOM	2007	0	LEU			67.703	48.634	15.128		22.62	0
ATOM	2007	СВ	LEU			70.041	49.875	16.192		23.11	C
ATOM	2009	CG	LEU			71.131	49.897	17.270		23.70	C
ATOM	2010		LEU			71.193	48.542	17.966		23.80	c
ATOM	2011		LEU			72.476	50.200	16.625		23.63	C
ATOM	2012	N	GLY			67.382	50.830	14.614		22.74	N
ATOM	2013	CA	GLY			66.576	50.655	13.419		24.26	C
ATOM	2014	C	GLY			67.414	50.872	12.172		24.94	C
ATOM	2015	0			381	67.648	49.946	11.397		25.50	0
ATOM	2016	N	ARG			67.882	52.103	11.992		26.09	N
ATOM	2017	CA	ARG			68.694	52.477	10.836		27.52	C
ATOM	2018	С	ARG			69.891	51.551	10.630		27.04	C
MOTA	2019	0	ARG			70.180	51.130	9.507		26.49	0
MOTA	2020	CB	ARG			69.199	53.911	10.998		29.77	C
MOTA	2021	CG			382	69.830	54.488	9.737	1.00	34.03	C
MOTA	2022	CD	ARG	Α	382	70.702	55.699	10.034	1.00	37.28	C
MOTA	2023	NE	ARG	A	382	72.102	55.327	10.247	1.00	41.27	N
ATOM	2024	CZ	ARG	Α	382	72.554	54.651	11.300	1.00	42.49	C
MOTA	2025	NHl	ARG	Α	382	71.723	54.267	12.255	1.00	44.24	N
MOTA	2026	NH2	ARG	Α	382	73.842	54.354	11.396	1.00	44.03	N
ATOM	2027	N	TYR	A	383	70.589	51.248	11.721	1.00	26.34	N
ATOM	2028	CA	TYR	A	383	71.763	50.380	11.679	1.00	25.33	C
MOTA	2029	C	TYR	A	383	71.493	49.062	10.948		24.88	C
ATOM	2030	0	TYR			72.280	48.639	10.096		24.77	0
ATOM	2031	CB	TYR			72.233	50.075	13.105		24.87	C
ATOM	2032	CG	TYR			73.466	49.203	13.179		24.53	С
MOTA	2033	CD1	-TYR	A	383	74.742	49.754	13.066	1.00	24.66	С

ATOM	2034	CD2	TYR	A	383	73.356	47.823	13.354	1.00 24.92	С
MOTA	2035	CE1	TYR	A	383	75.882	48.952	13.126	1.00 24.58	C
MOTA	2036	CE2	TYR	А	383	74.491	47.008	13.413	1.00 24.77	С
ATOM	2037	CZ	TYR	A	383	75.748	47.581	13.299	1.00 25.09	С
MOTA	2038	OH	TYR	Α	383	76.867	46.782	13.350	1.00 24.41	0
ATOM	2039	N	PHE	A	384	70.383	48.416	11.291	1.00 24.06	N
ATOM	2040	CA	PHE	Α	384	70.015	47.136	10.694	1.00 23.93	С
MOTA	2041	C	PHE	Α	384	69.289	47.263	9.357	1.00 24.44	С
MOTA	2042	0	PHE	Α	384	69.320	46.338	8.542	1.00 24.13	0
ATOM	2043	CB	PHE	Α	384	69.139	46.334	11.663	1.00 23.18	С
MOTA	2044	CG			384	69.869	45.847	12.889	1.00 22.86	С
MOTA	2045	CD1	PHE	Α	384	70.813	44.828	12.795	1.00 22.67	C
MOTA	2046		PHE			69.606	46.407	14.139	1.00 22.33	С
MOTA	2047	CE1	PHE	Ά	384	71.487	44.369	13.929	1.00 22.64	C
ATOM	2048		PHE			70.272	45.958	15.281	1.00 21.84	C
MOTA	2049	CZ			384	71.216	44.936	15.176	1.00 22.26	C
MOTA	2050	N			385	68.629	48.395	9.138	1.00 24.36	N
ATOM	2051	CA	ALA	Α	385	67.904	48.612	7.889	1.00 26.01	C
MOTA	2052	C	ALA	Α	385 .	68.839	48.544	6.679	1.00 26.76	С
MOTA	2053	. 0	ALA	Α	385	68.424	48.166	5.588	1.00 27.26	0
MOTA	2054	CB	ALA	Α	385	67.193	49.964	7.927	1.00 25.65	С
MOTA	2055	N	ARG	A	386	70.102	48.908	6.891	1.00 28.04	N
MOTA	2056	CA	ARG	Α	386	71.119	48.915	5.837	1.00 28.74	С
ATOM	2057	C	ARG	Α	386	71.531	47.529	5.344	1.00 28.88	C
MOTA	2058	0	ARG	Α	386	72.116	47.401	4.267	1.00 29.00	0
ATOM	2059	CB	ARG	Α	386	72.390	49.612	6.331	1.00 29.46	. C
MOTA	2060	CG	ARG	Α	386	72.241	51.044	6.813	1.00 31.77	С
MOTA	2061	CD	ARG	Α	386	73.547	51.470	7.482	1.00 32.99	С
ATOM	2062	NE	ARG	Α	386	73.922	50.500	8.508	1.00 34.12	N
ATOM	2063	CZ	ARG	Α	386	75.170	50.218	8.871	1.00 34.01	C
ATOM	2064	NH1	ARG	Α	386	76.197	50.830	8.294	1.00 33.31	N
MOTA	2065	NH2	ARG	Α	386	75.388	49.313	9.813	1:00 34.05	N
MOTA	2066	N	PHE	Α	387	71.239	46.495	6.127	1.00 28.95	N
ATOM	2067	CA	PHE	Α	387	71.649	45.146	5.763	1.00 28.84	C
ATOM	2068	C	PHE	Α	387 .	70.775	44.388	4.777	1.00 29.75	C
ATOM	2069	0	PHE	Α	387	69.581	44.642	4.641	1.00 29.59	0
ATOM	2070	CB	PHE	Α	387	71.833	44.289	7.021	1.00 28.17	С
MOTA	2071	CG	PHE	Α	387	72.742	44.904	8.050	1.00 28.00	C
ATOM	2072	CD1	PHE	Α	387	73.851	45.655	7.663	1.00 27.77	C
ATOM	2073	CD2	PHE	Α	387	72.499	44.723	9.408	1.00 27.53	C
ATOM	2074	CE1	PHE	Α	387	74.703	46.218	8.617	1.00 27.95	 C
MOTA	2075	CE2	PHE	A	387	73.346	45.282	10.370	1.00 26.97	C
MOTA	2076.	CZ	PHE	A	387	74.445	46.029	9.976	1.00 27.00	C
MOTA	2077	N	GLU	Α	388	71.412	43.441	4.100	1.00 30.90	N
ATOM	2078	CA	GLU	Α	388	70.773	42.585	3.112	1.00 32.08	C
ATOM	2079	C	GLU	Α	388	69.544	41.898	3.691	1.00 31.92	С
ATOM	2080	0	GLU	A	388	68.539	41.713	3.001	1.00 31.55	0
ATOM	2081	CB	GLU	Α	388	71.778	41.529	2.647	1.00 33.36	C
ATOM	2082	CG	GLU	Α	388	71.235	40.528	1.647	1.00 37.10	C
ATOM	2083	CD	GLU	A	388	70.777	41.189	0.367	1.00 38.82	С
ATOM	2084	OE1	GLU	A	388	71.594	41.898	-0.258	1.00 40.61	0
ATOM	2085	OE2	GLU	Α	388	69.604	41.000	-0.015	1.00 41.01	0
ATOM	2086	N	GLU	Α	389	69.626	41.532	4.967	1.00 31.81	N
ATOM	2087	CA			389	68.534	40.837	5.633	1.00 31.88	С
MOTA	2088	С	GLU	Α	389	67.315	41.667	6.027	1.00 31.91	С
ATOM	2089	0			389	66.307	41.103	6.442	1.00 31.96	0
MOTA	2090	CB			389	69.064	40.090	6.863	1.00 31.96	C

ATOM 2091 CG GLU A 389 71.527 39.515 6.562 1.00 31.96 ATOM 2092 CD GLU A 389 71.527 39.515 6.566 1.00 31.52 ATOM 2093 OEI GLU A 389 71.764 40.735 6.447 1.00 32.44 ATOM 2094 OEZ GLU A 389 72.431 38.676 6.715 1.00 32.24 ATOM 2095 N SER A 390 67.385 42.991 5.920 1.00 32.24 ATOM 2096 CA SER A 390 66.215 43.792 6.270 1.00 32.25 ATOM 2097 C SER A 390 66.5147 43.453 5.218 1.00 34.01 ATOM 2098 O SER A 390 65.147 43.453 5.218 1.00 34.01 ATOM 2098 O SER A 390 65.474 43.169 4.064 1.00 33.16 ATOM 2099 CB SER A 390 66.544 45.290 6.264 1.00 33.16 ATOM 2090 CB SER A 390 66.544 45.290 6.264 1.00 33.16 ATOM 2010 OG SER A 390 66.544 45.290 4.064 1.00 33.16 ATOM 2010 OG SER A 390 66.544 45.290 3.681 1.00 34.07 ATOM 2010 OG SER A 390 66.544 45.290 3.681 1.00 34.79 ATOM 2101 N PRO A 391 62.322 44.209 3.681 1.00 34.79 ATOM 2102 CA PRO A 391 62.322 44.209 3.681 1.00 34.79 ATOM 2103 C PRO A 391 62.322 44.209 3.681 1.00 35.94 ATOM 2105 CB PRO A 391 61.208 44.153 3.167 1.00 38.09 ATOM 2105 CB PRO A 391 61.850 43.944 6.725 1.00 34.53 ATOM 2107 CD PRO A 391 61.850 43.944 6.725 1.00 34.53 ATOM 2107 CD PRO A 391 61.850 43.944 6.725 1.00 34.53 ATOM 2107 CD PRO A 391 63.863 43.892 6.933 1.00 34.40 ATOM 2100 C PRO A 391 63.363 43.892 6.933 1.00 34.70 ATOM 2100 C THR A 392 63.196 45.157 3.373 1.00 38.30 ATOM 2100 C THR A 392 64.460 45.151 0.969 1.00 40.81 ATOM 2110 C THR A 392 64.460 45.151 0.969 1.00 40.81 ATOM 2111 O THR A 392 64.460 45.151 0.969 1.00 40.81 ATOM 2112 CB THR A 392 64.460 45.151 0.969 1.00 40.81 ATOM 2113 CG THR A 392 64.460 45.151 0.969 1.00 40.81 ATOM 2113 CG THR A 392 64.460 45.151 0.969 1.00 40.81 ATOM 2114 CG THR A 392 64.460 45.151 0.969 1.00 40.81 ATOM 2115 C A ARG A 393 63.100 47.581 2.920 1.00 39.79 ATOM 2115 C A ARG A 393 63.100 47.581 2.920 1.00 39.79 ATOM 2115 C A ARG A 393 63.100 47.581 2.920 1.00 39.79 ATOM 2115 C A ARG A 393 63.100 47.581 2.920 1.00 40.81 ATOM 2120 CG ARG A 393 63.100 47.54 4.259 1.00 44.65 ATOM 2121 CD ARG A 393 63.100 47.54 4.259 1.00 44.65 ATOM 2121 CD ARG A 393 63.100 47.54 4.259 1.00 44.66 A												
ATOM 2094 OBE GLU A 3899 71.764 40.735 6.447 1.00 32.44 ATOM 2094 OBE GLU A 3899 72.431 38.676 6.715 1.00 32.19 ATOM 2095 N SER A 390 67.385 42.991 5.920 1.00 32.19 ATOM 2095 CA SER A 390 66.215 43.792 6.270 1.00 32.24 ATOM 2097 C SER A 390 65.147 43.453 5.218 1.00 34.01 ATOM 2098 OBER A 390 65.147 43.453 5.218 1.00 34.01 ATOM 2098 OBER A 390 65.147 43.453 5.218 1.00 34.01 ATOM 2099 CB SER A 390 66.544 45.290 6.264 1.00 33.16 ATOM 2090 CB SER A 390 66.544 45.290 6.264 1.00 33.16 ATOM 2010 OG SER A 390 66.544 45.290 6.264 1.00 33.16 ATOM 2101 N PRO A 391 62.327 43.165 4.713 1.00 34.97 ATOM 2102 CA PRO A 391 62.322 44.209 3.661 1.00 34.79 ATOM 2102 CA PRO A 391 62.322 44.209 3.661 1.00 34.79 ATOM 2105 CB PRO A 391 61.208 44.153 3.167 1.00 38.09 ATOM 2105 CB PRO A 391 61.208 44.153 3.167 1.00 38.09 ATOM 2105 CB PRO A 391 61.850 43.944 6.725 1.00 34.53 ATOM 2107 CD PRO A 391 61.850 43.944 6.725 1.00 34.53 ATOM 2107 CD PRO A 391 63.363 43.892 6.933 1.00 34.40 ATOM 2108 N THR A 392 63.551 45.958 1.002 3.78 ATOM 2105 CB PRO A 391 63.363 43.892 6.933 1.00 34.40 ATOM 2108 N THR A 392 63.551 45.958 1.0072 1.00 41.04 ATOM 2103 CB THR A 392 63.551 45.958 1.0072 1.00 40.81 ATOM 2103 CB THR A 392 63.551 45.958 1.0072 1.00 40.81 ATOM 2113 CB THR A 392 64.460 45.131 0.969 1.00 40.81 ATOM 2113 CB THR A 392 64.629 47.674 3.085 1.00 40.84 ATOM 2113 CG THR A 392 64.629 47.674 3.085 1.00 40.84 ATOM 2115 CB THR A 392 64.620 47.674 3.085 1.00 40.84 ATOM 2115 CB THR A 392 64.620 47.674 3.085 1.00 40.81 ATOM 2115 CB THR A 393 63.707 46.556 -1.271 1.00 44.24 ATOM 2115 CB THR A 393 63.707 46.556 -1.271 1.00 44.25 ATOM 2115 CB ARG A 393 65.072 47.674 -1.372 1.00 44.85 ATOM 2115 CB ARG A 393 65.072 47.674 -1.372 1.00 44.85 ATOM 2115 CB ARG A 393 63.707 46.556 -1.271 1.00 44.28 ATOM 2115 CB ARG A 393 65.072 47.214 -1.372 1.00 44.85 ATOM 2120 CG ARG A 393 66.971 49.068 -1.237 1.00 49.97 ATOM 2121 CD ARG A 393 66.971 49.068 -1.237 1.00 46.86 ATOM 2131 CB ARG A 393 66.971 49.068 -1.237 1.00 46.87 ATOM 2132 CD LYS A 394 69.744 40.366 -2.258 1.0	MOTA	2091	CG	GLU	A	389	70.09	2 39.016	6.523	1.00 31.96		C
ATOM 2093 OEL GLU A 3899 72.431 38.676 6.447 1.00 32.19 ATOM 2094 OE2 GLU A 3899 72.431 38.676 6.715 1.00 32.19 ATOM 2095 N SER A 390 67.385 42.991 5.920 1.00 32.19 ATOM 2096 CA SER A 390 66.215 43.792 6.270 1.00 32.24 ATOM 2097 C SER A 390 65.147 43.453 5.218 1.00 34.01 ATOM 2098 O SER A 390 65.147 43.453 5.218 1.00 34.01 ATOM 2099 CB SER A 390 65.547 43.165 6.264 1.00 33.16 ATOM 2100 OG SER A 390 66.564 45.290 6.264 1.00 33.16 ATOM 2101 N PRO A 391 63.860 43.484 5.290 6.264 1.00 33.16 ATOM 2102 CA PRO A 391 62.322 44.209 3.681 1.00 34.72 ATOM 2103 C PRO A 391 62.322 44.209 3.681 1.00 35.94 ATOM 2105 CB PRO A 391 61.201 44.153 3.167 1.00 38.09 ATOM 2105 CB PRO A 391 61.201 44.153 3.167 1.00 38.09 ATOM 2105 CB PRO A 391 61.850 44.153 3.167 1.00 34.53 ATOM 2107 CD PRO A 391 61.850 44.153 3.167 1.00 34.53 ATOM 2108 C THR A 392 63.864 45.153 3.167 1.00 34.53 ATOM 2109 CB FRO A 391 63.363 43.892 6.933 1.00 34.40 ATOM 2108 C THR A 392 63.854 46.185 2.403 1.00 39.78 ATOM 2109 CA THR A 392 63.551 45.958 1.007 2 1.00 41.04 ATOM 2101 C THR A 392 64.460 45.131 0.969 1.00 40.81 ATOM 2110 C THR A 392 64.460 45.131 0.969 1.00 40.81 ATOM 2110 C THR A 392 64.629 47.674 3.085 1.00 40.34 ATOM 2110 C THR A 392 64.629 47.674 3.085 1.00 40.39.79 ATOM 2110 C THR A 392 64.629 47.674 3.085 1.00 40.39.79 ATOM 2110 C THR A 392 64.629 47.674 3.085 1.00 40.39.79 ATOM 2110 C THR A 392 64.629 47.674 3.085 1.00 40.91 ATOM 2111 C THR A 392 64.629 47.674 3.085 1.00 40.91 ATOM 2112 CB THR A 393 65.072 47.674 5.125 1.00 44.24 ATOM 2113 CG THR A 393 65.072 47.674 5.125 1.00 44.24 ATOM 2114 CGZ THR A 393 65.072 47.214 -1.372 1.00 44.65 ATOM 2115 N ARG A 393 65.072 47.214 -1.372 1.00 44.65 ATOM 2121 CD ARG A 393 65.072 47.214 -1.372 1.00 44.85 ATOM 2121 CD ARG A 393 65.072 47.214 -1.372 1.00 44.65 ATOM 2121 CD ARG A 393 66.971 49.086 -4.253 1.00 49.97 ATOM 2121 CD ARG A 393 66.971 49.086 -4.253 1.00 49.97 ATOM 2122 NE ARG A 393 66.971 49.086 -4.255 1.00 49.87 ATOM 2123 CD LYS A 394 66.971 47.866 -2.258 1.00 46.67 ATOM 2135 CD LYS A 394 66.913 49.9	ATOM	2092	CD	GLU	Α	389	71.52	7 39.515				C
ATOM 2095 N SER A 390 67.385 42.991 5.920 1.00 32.219 ATOM 2095 N SER A 390 66.215 43.792 6.270 1.00 33.25 ATOM 2097 C SER A 390 66.215 43.792 6.270 1.00 33.25 ATOM 2098 O SER A 390 65.147. 43.453 5.218 1.00 34.01 ATOM 2098 C SER A 390 65.147. 43.453 5.218 1.00 34.01 ATOM 2099 C SER A 390 65.447 43.169 4.064 1.00 33.38 ATOM 2099 C SER A 390 66.544 45.290 6.264 1.00 33.16 ATOM 2100 OG SER A 390 66.764 45.796 4.954 1.00 34.01 ATOM 2101 N PRO A 391 63.860 43.484 5.604 1.00 34.79 ATOM 2102 CA PRO A 391 62.322 44.209 3.681 1.00 35.94 ATOM 2103 C PRO A 391 62.322 44.209 3.681 1.00 37.25 ATOM 2104 O PRO A 391 61.208 44.153 3.167 1.00 38.09 ATOM 2105 CB PRO A 391 61.208 44.153 5.697 1.00 34.53 ATOM 2106 CG PRO A 391 61.850 43.944 6.725 1.00 34.53 ATOM 2107 CD PRO A 391 63.363 43.894 6.725 1.00 34.53 ATOM 2108 N THR A 392 63.196 45.157 3.373 1.00 38.30 ATOM 2109 CA THR A 392 63.196 45.157 3.373 1.00 38.30 ATOM 2101 C THR A 392 63.510 45.958 1.072 1.00 41.04 ATOM 2111 O THR A 392 63.510 47.581 0.999 1.00 40.81 ATOM 2112 CB THR A 392 63.210 47.581 0.999 1.00 40.81 ATOM 2113 OGITHR A 392 63.207 47.574 3.2920 1.00 39.78 ATOM 2116 CA ARG A 393 65.707 46.566 -1.271 1.00 44.24 ATOM 2117 C ARG A 393 65.306 48.298 -0.834 1.00 49.34 ATOM 2116 CA ARG A 393 65.070 47.574 1.372 1.00 44.24 ATOM 2117 C ARG A 393 65.070 47.574 1.372 1.00 44.24 ATOM 2118 O ARG A 393 65.070 47.574 1.372 1.00 44.24 ATOM 2119 CB ARG A 393 65.070 47.574 1.372 1.00 44.24 ATOM 2110 C THR A 392 64.609 47.674 3.085 1.00 49.97 ATOM 2120 CG ARG A 393 65.070 47.574 1.372 1.00 44.24 ATOM 2111 O ARG A 393 65.070 47.574 1.372 1.00 44.24 ATOM 2112 CB THR A 392 64.609 47.674 3.085 1.00 49.97 ATOM 2120 CG ARG A 393 65.070 47.574 47.144 1.372 1.00 44.24 ATOM 2121 CD ARG A 393 65.070 47.574 47.144 1.372 1.00 44.24 ATOM 2121 CD ARG A 393 65.070 47.574 47.144 1.372 1.00 44.24 ATOM 2121 CD ARG A 393 65.070 47.574 47.144 1.372 1.00 44.65 ATOM 2122 NE ARG A 393 65.070 47.574 47.144 1.372 1.00 44.65 ATOM 2130 CF LYS A 394 67.309 47.056 -2.296 1.00 45.87 ATOM 2123 CD LYS A 394 6	ATOM	2093	OE1	GLU	Α	389	71.76					ō
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ATOM 2118 O ARG A 393 65.306 48.298 -0.834 1.00 44.87 ATOM 2119 CB ARG A 393 62.806 47.196 -2.337 1.00 45.06 ATOM 2120 CG ARG A 393 61.425 46.587 -2.464 1.00 46.87 ATOM 2121 CD ARG A 393 60.966 46.622 -3.919 1.00 48.41 ATOM 2122 NE ARG A 393 60.966 46.622 -3.919 1.00 48.41 ATOM 2123 CZ ARG A 393 60.971 49.068 -4.253 1.00 49.97 ATOM 2124 NH1 ARG A 393 60.138 49.231 -3.233 1.00 50.58 ATOM 2125 NH2 ARG A 393 61.410 50.125 -4.925 1.00 50.58 ATOM 2126 N LYS A 394 66.911 50.125 -4.925 1.00 50.50 ATOM 2128 C LYS A 394 66.911 47.242 -4.645 1.00 46.21 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 45.89 ATOM 2130 CB LYS A 394 66.911 47.242 -4.645 1.00 45.89 ATOM 2131 CG LYS A 394 66.914 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.64 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.64 ATOM 2134 NZ LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2135 CA VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2137 C VAL A 395 67.316 49.977 -4.726 1.00 48.01 ATOM 2139 CB VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2134 CG TAL A 395 66.473 52.014 -3.435 1.00 48.06 ATOM 2137 C VAL A 395 66.473 52.014 -3.435 1.00 48.03 ATOM 2130 CB VAL A 395 66.473 52.014 -3.435 1.00 49.08 ATOM 2131 CG TAL A 395 66.473 52.014 -3.435 1.00 49.08 ATOM 2134 CA THR A 396 69.691 52.708 -7.835 1.00 49.73 ATOM 2144 C THR A 396 69.697 52.759 8.516 1.00 50.30 ATOM 2144 C THR A 396 69.607 52.759 8.516 1.00 50.30 ATOM 2144 C THR A 396 69.607 52.759 8.516 1.00 50.30		2116	CA	ARG	A	393	63.70	7 46.566	-1.271	1.00 44.24		С
ATOM 2119 CB ARG A 393 62.806 47.196 -2.337 1.00 45.06 ATOM 2120 CG ARG A 393 61.425 46.587 -2.464 1.00 46.87 ATOM 2121 CD ARG A 393 60.966 46.622 -3.919 1.00 48.41 ATOM 2122 NE ARG A 393 60.966 46.622 -3.919 1.00 49.42 ATOM 2123 CZ ARG A 393 60.971 49.068 -4.253 1.00 49.97 ATOM 2124 NH1 ARG A 393 60.138 49.231 -3.233 1.00 50.58 ATOM 2125 NH2 ARG A 393 60.138 49.231 -3.233 1.00 50.58 ATOM 2126 N LYS A 394 65.973 46.535 -2.069 1.00 45.28 ATOM 2127 CA LYS A 394 67.309 47.056 -22.96 1.00 46.21 ATOM 2128 C LYS A 394 66.911 47.833 -3.598 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2131 CG LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.64 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.64 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.64 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.64 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.66 ATOM 2133 CE LYS A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.67 ATOM 2138 O VAL A 395 66.086 51.049 -4.543 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.475 50.379 -4.223 1.00 48.03 ATOM 2140 CG1 VAL A 395 66.086 51.049 -4.543 1.00 49.08 ATOM 2141 CG2 VAL A 395 66.075 50.379 -4.223 1.00 48.03 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2143 CA THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 50.30	ATOM	2117	C	ARG	Α	393	65.07	2 47.214	-1.372	1.00 44.65		С
ATOM 2120 CG ARG A 393 61.425 46.587 -2.464 1.00 46.87 ATOM 2121 CD ARG A 393 60.966 46.622 -3.919 1.00 48.41 ATOM 2122 NE ARG A 393 61.374 47.850 -4.597 1.00 49.42 ATOM 2123 CZ ARG A 393 60.971 49.068 -4.253 1.00 49.97 ATOM 2124 NH1 ARG A 393 60.138 49.231 -3.233 1.00 50.58 ATOM 2125 NH2 ARG A 393 61.410 50.125 -4.925 1.00 50.50 ATOM 2126 N LYS A 394 65.973 46.535 -2.069 1.00 45.28 ATOM 2127 CA LYS A 394 67.309 47.056 -2.296 1.00 46.21 ATOM 2128 C LYS A 394 66.911 47.833 -3.598 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 66.911 47.242 -4.645 1.00 45.89 ATOM 2131 CG LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2132 CD LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.66 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.64 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.64 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.66 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.61 ATOM 2137 C VAL A 395 67.183 49.977 -4.726 1.00 48.61 ATOM 2138 O VAL A 395 66.086 51.049 -4.543 1.00 48.68 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.03 ATOM 2140 CG1 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2142 N THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2143 CA THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.759 -8.516 1.00 50.30	ATOM	2118	0				65.30	48.298	-0.834	1.00 44.87		0
ATOM 2121 CD ARG A 393 60.966 46.622 -3.919 1.00 48.41 ATOM 2122 NE ARG A 393 61.374 47.850 -4.597 1.00 49.42 ATOM 2123 CZ ARG A 393 60.971 49.068 -4.253 1.00 49.97 ATOM 2124 NH1 ARG A 393 60.138 49.231 -3.233 1.00 50.58 ATOM 2125 NH2 ARG A 393 61.410 50.125 -4.925 1.00 50.50 ATOM 2126 N LYS A 394 65.973 46.535 -2.069 1.00 45.28 ATOM 2127 CA LYS A 394 67.309 47.056 -2.296 1.00 46.21 ATOM 2128 C LYS A 394 67.171 47.833 -3.598 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.618 44.049 -2.140 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2137 C VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2138 CA VAL A 395 68.489 50.671 -5.078 1.00 48.67 ATOM 2139 CB VAL A 395 69.209 51.136 -4.197 1.00 48.67 ATOM 2139 CB VAL A 395 69.209 51.136 -4.197 1.00 48.67 ATOM 2131 CG VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2134 NZ NZ LYS A 394 70.618 4.757 50.379 -4.223 1.00 48.03 ATOM 2134 CG THR A 396 69.209 50.736 -6.831 1.00 47.99 ATOM 2140 CG1 VAL A 395 66.4757 50.379 -4.223 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.915 52.708 -7.493 1.00 49.08 ATOM 2144 C THR A 396 69.691 52.708 -7.835 1.00 49.70	ATOM	2119	CB ·	ARG	А	393	62.80	47.196	-2.337	1.00 45.06		С
ATOM 2122 NE ARG A 393 61.374 47.850 -4.597 1.00 49.42 ATOM 2123 CZ ARG A 393 60.971 49.068 -4.253 1.00 49.97 ATOM 2124 NH1 ARG A 393 60.138 49.231 -3.233 1.00 50.58 ATOM 2125 NH2 ARG A 393 61.410 50.125 -4.925 1.00 50.50 ATOM 2126 N LYS A 394 65.973 46.535 -2.069 1.00 45.28 ATOM 2127 CA LYS A 394 67.309 47.056 -2.296 1.00 46.21 ATOM 2128 C LYS A 394 67.171 47.833 -3.598 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 66.911 47.242 -4.645 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.54 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.54 ATOM 2134 NZ LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2137 C VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2138 C A VAL A 395 69.209 51.136 -4.197 1.00 48.01 ATOM 2139 CB VAL A 395 69.209 51.136 -4.197 1.00 48.06 ATOM 2139 CB VAL A 395 66.475 50.379 -4.223 1.00 48.06 ATOM 2134 CG VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2134 CG VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2134 CG THR A 396 69.209 50.376 -6.370 1.00 49.08 ATOM 2140 CG1 VAL A 395 66.475 50.379 -4.223 1.00 49.08 ATOM 2140 CG1 VAL A 395 66.91 52.708 -7.493 1.00 49.08 ATOM 2144 C THR A 396 69.691 52.708 -7.835 1.00 49.70	MOTA	2120	CG	ARG	A	393	61.429	46.587	-2.464	1.00 46.87		C
ATOM 2123 CZ ARG A 393 60.971 49.068 -4.253 1.00 49.97 ATOM 2124 NH1 ARG A 393 60.138 49.231 -3.233 1.00 50.58 ATOM 2125 NH2 ARG A 393 61.410 50.125 -4.925 1.00 50.50 ATOM 2126 N LYS A 394 65.973 46.535 -2.069 1.00 45.28 ATOM 2127 CA LYS A 394 67.309 47.056 -2.296 1.00 46.21 ATOM 2128 C LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 66.911 47.242 -4.645 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.66 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2137 C VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2138 O VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2141 CG2 VAL A 395 66.475 50.379 -4.223 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 49.98 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.30 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30	MOTA	2121	CD	ARG	Α	393	60.96	46.622	-3.919	1.00 48.41		С
ATOM 2124 NH1 ARG A 393 60.138 49.231 -3.233 1.00 50.58 ATOM 2125 NH2 ARG A 393 61.410 50.125 -4.925 1.00 50.50 ATOM 2126 N LYS A 394 65.973 46.535 -2.069 1.00 45.28 ATOM 2127 CA LYS A 394 67.309 47.056 -2.296 1.00 46.21 ATOM 2128 C LYS A 394 66.911 47.242 -4.645 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 66.911 47.242 -4.645 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 69.744 46.366 -2.558 1.00 46.46 ATOM 2133 CE LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2137 C VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2138 O VAL A 395 69.209 51.136 -4.197 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.086 51.049 -4.543 1.00 48.03 ATOM 2140 CG1 VAL A 395 66.475 50.379 -4.223 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.475 50.379 -4.223 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.475 50.379 -4.223 1.00 49.08 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 50.30	ATOM	2122	NE	ARG	Α	393	61.374	47.850	-4.597	1.00 49.42		N
ATOM 2125 NH2 ARG A 393 61.410 50.125 -4.925 1.00 50.50 ATOM 2126 N LYS A 394 65.973 46.535 -2.069 1.00 45.28 ATOM 2127 CA LYS A 394 67.309 47.056 -2.296 1.00 46.21 ATOM 2128 C LYS A 394 67.171 47.833 -3.598 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2138 O VAL A 395 66.489 50.671 -5.078 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.473 52.014 -3.435 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2143 CA THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 49.70	ATOM	2123	CZ	ARG	Α	393	60.97	L 49.068	-4.253	1.00 49.97		С
ATOM 2126 N LYS A 394 65.973 46.535 -2.069 1.00 45.28 ATOM 2127 CA LYS A 394 67.309 47.056 -2.296 1.00 46.21 ATOM 2128 C LYS A 394 67.171 47.833 -3.598 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 66.086 51.049 -4.543 1.00 48.67 ATOM 2139 CB VAL A 395 66.475 50.379 -4.223 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.475 50.379 -4.223 1.00 47.99 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 49.70	MOTA	2124	NH1	ARG	A	393	60.138	3 49.231	-3.233	1.00 50.58		N
ATOM 2126 N LYS A 394 65.973 46.535 -2.069 1.00 45.28 ATOM 2127 CA LYS A 394 67.309 47.056 -2.296 1.00 46.21 ATOM 2128 C LYS A 394 67.171 47.833 -3.598 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 66.086 51.049 -4.543 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.475 50.379 -4.223 1.00 47.99 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 50.30	MOTA	2125	NH2	ARG	Α	393	61.410	50.125	-4.925	1.00 50.50		N
ATOM 2128 C LYS A 394 67.309 47.056 -2.296 1.00 46.21 ATOM 2128 C LYS A 394 67.171 47.833 -3.598 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2137 C VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2138 O VAL A 395 66.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2143 CA THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 70.770 50.497 -7.835 1.00 49.70	MOTA	2126	N	LYS	Α	394	65.973	3 46.535				N
ATOM 2128 C LYS A 394 67.171 47.833 -3.598 1.00 46.79 ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 66.086 51.049 -4.543 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.086 51.049 -4.543 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2143 CA THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 50.30	ATOM	2127	CA									С
ATOM 2129 O LYS A 394 66.911 47.242 -4.645 1.00 47.04 ATOM 2130 CB LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 69.209 51.136 -4.197 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.086 51.049 -4.543 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.475 50.379 -4.223 1.00 48.03 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2143 CA THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 70.770 50.497 -7.835 1.00 49.70	ATOM	2128	С	LYS	Α	394						C
ATOM 2130 CB LYS A 394 68.304 45.913 -2.478 1.00 45.89 ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 66.086 51.049 -4.543 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2143 CA THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 70.770 50.497 -7.835 1.00 49.70	ATOM		0	LYS	A	394						ō
ATOM 2131 CG LYS A 394 69.744 46.366 -2.558 1.00 46.14 ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 69.209 51.136 -4.197 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 66.4757 50.379 -4.223 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.4757 50.379 -4.223 1.00 47.99 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2143 CA THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 70.770 50.497 -7.835 1.00 49.70	ATOM	2130	СВ									C
ATOM 2132 CD LYS A 394 70.649 45.254 -3.055 1.00 46.46 ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 69.209 51.136 -4.197 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 64.757 50.379 -4.223 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2143 CA THR A 396 68.792 50.736 -6.370 1.00 49.73 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 70.770 50.497 -7.835 1.00 49.70										_		C
ATOM 2133 CE LYS A 394 70.618 44.049 -2.140 1.00 46.54 ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 69.209 51.136 -4.197 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 64.757 50.379 -4.223 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 70.770 50.497 -7.835 1.00 49.70										-		C
ATOM 2134 NZ LYS A 394 71.498 42.968 -2.658 1.00 46.60 ATOM 2135 N VAL A 395 67.316 49.151 -3.533 1.00 47.31 ATOM 2136 CA VAL A 395 67.183 49.977 -4.726 1.00 48.01 ATOM 2137 C VAL A 395 68.489 50.671 -5.078 1.00 48.58 ATOM 2138 O VAL A 395 69.209 51.136 -4.197 1.00 48.67 ATOM 2139 CB VAL A 395 66.086 51.049 -4.543 1.00 48.06 ATOM 2140 CG1 VAL A 395 64.757 50.379 -4.223 1.00 48.03 ATOM 2141 CG2 VAL A 395 66.473 52.014 -3.435 1.00 47.99 ATOM 2142 N THR A 396 68.792 50.736 -6.370 1.00 49.08 ATOM 2143 CA THR A 396 68.792 50.736 -6.831 1.00 49.73 ATOM 2144 C THR A 396 69.691 52.708 -7.493 1.00 50.27 ATOM 2145 O THR A 396 69.007 52.759 -8.516 1.00 50.30 ATOM 2146 CB THR A 396 70.770 50.497 -7.835 1.00 49.70												C
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												0
71.053 49.228 -7.234 1.00 49.67												C
	ATON	4 1 4 1	061	ınk	H	330	/1.053	47.228	-1.234	1.00 49.67		0

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ATOM	2148	CG2	THR			72.080	51.159	-8.240	1.00	49.85		С
ATOM	2149	N	ILE	Α	397	70.192	53.784	-6.899	1.00	50.84		N
ATOM	2150	CA	ILE	Α	397	69.953	55.122	-7.416	1.00	51.13		C
ATOM	2151	C	ILE	Α	397	71.261	55.795	-7.821	1.00	51.21		С
ATOM	2152	0	ILE	Α	39 <b>7</b>	72.043	56.214	-6.967		51.47		0
ATOM	2153	CB			397	69.260	56.001	-6.358		51.32		Ċ
ATOM	2154	CG1	ILE								•	C
						68.033	55.276	-5.800		51.51		
MOŢA	2155	CG2	ILE			68.855	57.333	-6.977		51.27		С
ATOM	2156	CD1				67.325	56.029	-4.691		51.49		С
ATOM	2157	N	ASN			71.49 <b>7</b>	55.889	-9.126	1.00	51.17		N
ATOM	2158	CA	ASN	Α	398	72.702	56.528	-9.644	1.00	50.97		С
MOTA	2159	C	ASN	Α	398	73.987	55.852	-9.174	1.00	50.29		С
ATOM	2160	0	ASN	Α	398	74.930	56.525	-8.758	1.00	50.58		0
ATOM	2161	CB	ASN			72.730	58.000	-9.228		51.92		C
ATOM	2162	CG	ASN			71.476	58.742	-9.635		52.91		C
ATOM	2163		ASN			71.150		-10.819		5363		o
ATOM	2164		ASN			70.761	59.284	-8.654		53.34		
											•	N
ATOM	2165	N	GLY			74.021.	54.526	-9.238		49.43		N
ATOM	2166	CA	GLY			75.209	53.801	-8.824		48.10		С
ATOM	2167	С	GLY			75.308	53.532	-7.334		47.22		C
MOTA	2168	0	GLY	Α	399	76.228	52.844	-6.887	1.00	47.45		0
MOTA	2169	N	SER	Α	400	74.374	54.073	-6.559	1.00	45.83		N
MOTA	2170	CA	SER	Α	400	74.387	53.864	-5.115	1.00	44.44		С
ATOM	2171	C	SER	A	400	73.287	52.916	-4.674	1.00	43.04		С
ATOM	2172	0	SER			72.100	53.221	-4.793	1.00	42.88		0
ATOM	2173	CB	SER			74.243	55.195	-4.373		44.67		C
ATOM	2174	OG	SER			75.455	55.926	-4.407		45.51		0
ATOM	2175		VAL									
		N				73.692	51.757	-4.167		41.55		N
ATOM	2176	CA	VAL			72.739	50.768	-3.697		40.15		C
ATOM	2177	C	VAL			72.251	51.225	-2.328		39.84		С
ATOM	2178	0	VAL			73.046	51.445	-1.413	1.00	39.36		0
MOTA	2179	CB	VAL	Α	401	73.395	49.375	-3.599	1.00	39.80		C
ATOM	2180	CG1	VAL	Α	401	72.386	48.348	-3.117	1.00	38.64		С
ATOM	2181	CG2	VAL	A	401	73.944	48.971	-4.966	1.00	39.24	•	С
MOTA	2182	N	MET	A	402	70.938	51.387	-2.206	1.00	39.55		N
MOTA	2183	CA	MET	Α	402	70.329	51.837	-0.961	1.00	39.09		С
	2184	С	MET			69.240	50.864	-0.539		38.02		C
ATOM	2185	Ō	MET			68.872	49.962	-1.289		37.68		0
ATOM	2186	СВ	MET			69.683						C
						_	53.213	-1.148		40.51		
ATOM	2187	CG	MET			70.529	54.244	-1.882		42.23		C
ATOM	2188	SD	MET				54.787	-0.942				S
ATOM	2189	CE	MET			71.204	56.039	0.120		43.68		C
ATOM	2190		LYS			68.734	51.059	0.673		36.46		N
MOTA	2191	CA	LYS			67.649	50.250	1.199		35.41		С
MOTA	2192	C	LYS	Α	403	66.641	51.227	1.785	1.00	34.75		C
ATOM	2193	0	LYS	Α	403	67.016	52.298	2.265	1.00	34.48		0
ATOM	2194	CB	LYS	Α	403	68.153	49.275	2.266	1.00	35.62		С
ATOM	2195	CG	LYS	Α	403	69.086	48.205	1.710	1.00	35.12		С
ATOM	2196	CD -	LYS			68.847	46.848	2.346	1.00	35.57		C
ATOM	2197	CE	LYS			67.466	46.315	2.009		35.05		C
ATOM	2198	NZ	LYS			67.242	44.936	2.521		33.99		N
ATOM		NZ,										
	2199		GLU			65.364	50.869	1.727		34.23		N
ATOM	2200	CA	GLU			64.305	51.734	2.235		34.40	•	Ç
ATOM	2201	C	GLU			64.259	51.735	3.754		33.56		C
MOTA	2202	0	GLU			64.590	50.740	4.394		33.40		0
MOTA	2203	CB	GĽU	A	404	62.947	51.268	1.718	1.00	35.68		C
MOTA	2204	CG	GLU	А	404	62.879	51.034	0.225	1.00	38.04		С

MOTA	2205	CD	GLU	A	404	61.547	50.453	-0.193	1.00 39.70		С
MOTA	2206	OE1	GLU	Α	404	61.264	49.284	0.159	1.00 40.89		0
MOTA	2207	OE2	GLU	Α	404	60.778	51.171	-0.864	1.00 40.74		0
ATOM	2208	N	TYR	Α	405	63.833	52.855	4.325	1.00 32.74	•	N
MOTA	2209	CA	TYR	Α	405	63.714	52.975	5.770	1.00 32.04		C
ATOM	2210	C	TYR	A	405	62.665	54.027	6.092	1.00 31.67		C
ATOM	2211	0	TYR	Α	405	62.782	55.179	5.677	1.00 32.05		0
MOTA	2212	CB			405	65.059	53.365	6.392	1.00 31.13		C
ATOM	2213	CG			405	65.049	53.387	7.905	1.00 30.72		C
ATOM	2214	CD1			405	64.643	52.269	8.636	1.00 29.79		C
ATOM	2215	CD2			405	65.451	54.523	8.607	1.00 29.90		C
MOTA	2216	CE1			405	64.638	52.282	10.033	1.00 30.48		C
ATOM	2217	CE2			405	65.449	54.546	10.001	1.00 30.40		C
MOTA	2218	CZ			405	65.041	53.423	10.707	1.00 30.04		C
ATOM	2219	OH			405	65.029	53.448	12.085	1.00 30.22		
ATOM	2220	N			406	61.632	53.627	6.822	1.00 30.03		0
ATOM	2221	CA			406	60.574	54.555	7.186	1.00 31.08		N
ATOM	2222	C			406	6.0.134	54.345	8.629	1.00 30.89		C
ATOM	2223	:0			406	60.190	53.231	9.150			C
ATOM	2224	CB			406	59.384	54.401		1.00 30.22		0
ATOM	2225	CG			406	58.715	53.059	6.227 6.267	1.00 29.70		C
ATOM	2226	CD1			406	57.695			1.00 28.77		C
ATOM	2227	CD2				59.018	52.675	7.090	1.00 28.91		C
ATOM	2228	NE1	TRP			57.342	51.924	5.448	1.00 28.70		C
ATOM	2229	CE2	TRP				51.374	6.833	1.00 29.02		N
ATOM	2230	CE3	TRP			58.139 59.947	50.887	5.831	1.00.28.47		C
ATOM	2231	CZ2					51.681	4.426	1.00 28.73		C
ATOM	2232	CZ3	TRP			58.158	49.624	5.228	1.00 28.64		C
ATOM	2232	CH2				59.967	50.423	3.825	1.00 29.12	•	C
ATOM	2234	N	GLY			59.075	49.411	4.231	1.00 29.01		С
ATOM	2235	CA	GLY			59.708	55.428	9.270	1.00 31.77		N
ATOM	2236	CA	GLY			59.270	55.349	10.652	1.00 32.35		·C
ATOM	2237	0	GLY			57.927	54.665	10.816	1.00 32.51		С
ATOM						57.124	54.619	9.887	1.00 32.50		0
ATOM	2238 2239	N	GLU			57.685	54.125	12.005	1.00 32.68		N
		CA	GLU			56.428	53.450	12.296	1.00 32.74		C
ATOM	2240	С	GLU			55.302	54.465	12.443	1.00 33.30		C
ATOM ATOM	2241	0	GLU			54.127	54.106	12.447	1.00 33.00		0
ATOM	2242	CB	GLU			56.562	52.625	13.576	1.00 32.42		С
ATOM ·	2243	CG.	GLU			57.342	51.343	13.382	1.00 32.27		С
			GLU			56.618	50.373	12.460	1.00 32.10		С
MOTA	2245		GLU			55.511	49.930	12.824	1.00 31.95		0
ATOM	2246		GLU			57.149	50.059	11.376	1.00 31.80		0
ATOM	2247	N	GLY			55.670	55.736	12.563	1.00 34.53		·N
MOTA	2248	CA	GLY			54.677	56.784	12.702	1.00 36.36		Ç
ATOM	2249	C	GLY			54.250	57.358	11.362	1.00 37.80		C
ATOM	2250	0	GLY			53.313	58.148	11.291	1.00 37.85		0
ATOM	2251	N	SER			54.934	56.965	10.293	1.00 39.37		N
ATOM	2252	CA	SER			54.598	57.462	8.963	1.00 41.45		С
ATOM	2253	C	SER			53.291	56.839	8.485	1.00 43.20		C
ATOM	2254	0	SER			52.945	55.723	8.876	1.00 42.83		0
ATOM	2255	CB	SER			55.715	57.135	7.971	1.00 40.60		C
ATOM	2256	OG	SER			55.795	55.740	7.738	1.00 40.47		0
ATOM	2257	N	SER			52.564	57.566	7.642	1.00 45.39	•	N
ATOM	2258	CA	SER			51.300	57.065	7.120	1.00 47.54		С
ATOM	2259	C	SER			51.556	55.777	6.347	1.00 48.82		C
ATOM	2260	0	SER			50.699	54.897	6.287	1.00 48.87		0
ATOM	2261	CB	SER	A	411	50.642	58.113	6.212	1.00 47.83		C

MOTA	2262	OG	SER	Α	411	51.518	58.534	5.180	1.00	48.13		0
MOTA	2263	N	ARG	Α	412	52.750	55.669	5.770	1.00	50.57		N
MOTA	2264	CA	ARG	Α	412	53.125	54.483	5.009	1.00	52.38		С
MOTA	2265	С	ARG	Α	412	53.169	53.244	5.895	1.00	53.64		С
MOTA	2266	0	ARG	A	412	52.940	52.130	5.426	1.00	53.63		0
MOTA	2267	CB	ARG	A	412	54.495	54.677	4.351	1.00	52.24		С
ATOM	2268	CG	ARG	A	412	55.008	53.420	3.652	1.00	52.42		C
ATOM	2269	CD			412	56.351	53.628	2.971	1.00	52.24		С
ATOM	2270	NE			412	56.789	52.412	2.286	1.00			N
MOTA	2271	CZ			412	57.920	52.298	1.596	1.00		•	С
ATOM	2272	NHl	ARG			58.747	53.329	1.487	1.00			N
ATOM	2273 -		ARG			58.226	51.145	1.014	1.00			N
ATOM	2274	N			413	53.465	53.445	7.176	1.00			N
ATOM	2275	CA	ALA			53.555	52.344	8.128		57.35		C
MOTA	2276	C			413	52.196	51.934	8.682		58.87		Ċ
ATOM	2277	0			413	51.760	50.799	8.501	1.00			Ö
ATOM	2278	СВ			413	54.483	52.725	9.278	1.00			Ċ
	2279	N			414	51.532	52.858	9.368	1.00			N
ATOM	2280	CA			414	50.232	52.558	9.945	1.00			. C
ATOM	2281	C			414	49.102	52.862	8.968	1.00		v	C
ATOM	2282	Ō			414	48.824	54.018	8.648	1.00			Ö
ATOM	2283	СВ			414	50.040	53.330	11.259	1.00			C
ATOM	2284	CG			414	50.007	54.843	11.139	1.00			Ċ
ATOM	2285	CD			414	49.833	55.477	12.511	1.00			C
ATOM	2286	NE			414	49.344	56.850	12.427	1.00			N
ATOM	2287	CZ			414	49.075	57.614	13.481	1.00			C
ATOM	2288		ARG			49.250	57.143	14.709	1.00			N
ATOM	2289		ARG			48.615	58.846	13.311	1.00			N
ATOM	2290	N			415	48.467	51.799	8.486	1.00			N
ATOM	2291	CA	ASN			47.361	51.907	7.542	1.00			C
ATOM	2292	C			415	46.837	50.495	7.276	1.00			C
ATOM	2293	Ö			415	46.002	50.282	6.397	1.00			0
ATOM	2294	СВ			415	47.840	52.552	6.233	1.00			C
ATOM	2295	CG			415	46.701	53.155	5.418	1.00			C
ATOM	2296				415	45.788	52.454	4.978	1.00			0
MOTA	2297		ASN			46.756	54.466	5.215	1.00			N
ATOM	2298	N			416	47.343	49.534	8.045	1.00			N
ATOM	2299	CA	TRP			46.932	48.140	7.915	1.00			C
ATOM	2300 -				416	45.656	47.901	8.719	1.00			C
ATOM	2301	0			416	44.616	47.529	8.171	1.00			0.
ATOM	2302	CB			416	48.040	47.209	8.424	1.00			C
ATOM	2303	CG			416	48.339	47.382	9.886	1.00			C
ATOM	2304		TRP		•	49.047	48.397	10.465	1.00			C
ATOM	2305		TRP			47.868	46.558	10.960	1.00			C
ATOM	2306	NE1	TRP			49.040	48.259	11.834	1.00			N
ATOM	2307	CE2				48.323	47.139	12.164	1.00			C
ATOM	2308	CE3				47.101	45.388	11.021	1.00			C
ATOM	2309	CZ2				48.036	46.588	13.419	1.00			C
ATOM	2310	CZ3	TRP			46.815	44.839	12.268	1.00			C
ATOM	2311		TRP			47.282	45.441	13.450	1.00			C
ATOM	2312	N			430	49.118	63.275	11.644	1.00			N
ATOM	2312	CA	GLU			50.037	62.232	12.086	1.00			C
ATOM	2314	C			430	51.464	62.554	11.659	1.00			C
ATOM	2315	0			430	51.709	63.560	10.992	1.00			0
ATOM	2316	СВ	GLU			49.622	60.882	11.499	1.00			C
ATOM	2317	CG			430	49.622	60.809	9.981	1.00			C
ATOM	2317	CD	GLU			49.250	59.466	9.439	1.00			C
			0			17.230	22.400	٠٠٩٥٥	1.00			C

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MOTA	2319	OE1	GLU	Α	430	49.840	58.437	9.831	1.00	73.94		0
MOTA	2320	OE2	GLU	A	430	48.308	59.439	8.619	1.00	74.25		0
MOTA	2321	N	GLU	Α	431	52.403	61.695	12.046	1.00	71.87		N
MOTA	2322	CA	GLU	A	431	53.803	61.891	11.692	1.00	71.10		C
MOTA	2323	С	GLU	Α	431	54.066	61.249	10.333	1.00	70.43		С
MOTA	2324	0	GLU	Α	431	53.136	60.792	9.666	1.00	70.43		0
MOTA	2325	CB	GLU	A	431	54.714	61.254	12.744	1.00	71.29		C
MOTA	2326	CG	GLU	Α	431	56.138	61.783	12.716	1.00	71.71		C
ATOM	2327	CD	GLU	A	431	57.111	60.917	13.493	1.00	71.87		C
ATOM	2328	OE1	GLU			56.854	60.632	14.684	1.00	72.06		0
MOTA	2329	OE2	GLU			58.141	60.528	12.907	1.00	71.88		0
ATOM	2330	N			432	55.331	61.211	9.926	1.00	69.40		N
ATOM	2331	CA	GLY	Α	432	55.667	60.614	8.647	1.00	67.99		С
ATOM	2332	C ·	GLY			57.101	60.847	8.215	1.00	66.90		C
ATOM	2333	0	GLY			57.524	61.987	8.030		67.35	•	0
ATOM	2334	N	VAL			57.853	59.763	8.054		65.49		N
ATOM	2335	CA	VAL			59.246	59.851	7.631		63.66		C
ATOM	2336	C	VAL			59.611	58.651	6.760		62.12		Ċ
ATOM	2337	0	VAL			59.537	57.503	7.200		61.66		ō
MOTA	2338	CB	VAL			60.198	59.891	8.840		64.04		Ċ
ATOM	2339		VAL			61.624	60.100	8.366		64.18		C
ATOM	2340		VAL			59.784	60.994	9.797		64.08		C
	2341	N	ASP			60.008	58.930	5.522		60.25		N
ATOM	2341		ASP			60.377	57.892	4.566		58.26		C
ATOM		CA						3.947				
MOTA	2343	C	ASP			61.718	58.280			56.78		C.
ATOM	2344	0	ASP			61.881	59.405	3.475		56.70		0
ATOM	2345	CB	ASP			59.311	57.805	3.470		58.76		C
ATOM	2346	CG			434	59.280	56.456	2.783		58.92		C
MOTA	2347		ASP			60.357	55.902	2.487		59.73		0
	2348		ASP			58.168	55.955	2.525		59.23		0
MOTA	2349	N			435	62.676	57.359	3.944		54.66		N
MOTA	2350	CA			435	63.988	57.664	3.382		52.26		C
MOTA	2351	C			435	64.779	56.437	2.938		50.24		C
ATOM	2352	0			435	64.263	55.319	2.913		49.77		0
ATOM	2353	CB			435	64.815	58.454	4.400		52.83		С
MOTA	2354	OG			435	65.010	57.701	5.586	1.00	53.50		0
MOTA	2355	N			436	66.040	56.668	2.586		47.86		N
MOTA	2356	CA			436	66.935	55.609	2.140		45.83		C
MOTA	2357	C .			436	68.198	55.593	2.993		43.91		C
MOTA	2358	0	TYR	Α	436	68.622	56.626	3.513	1.00	43.83		0
MOTA	2359	CB	TYR	A	436	67.333	55.825	0.677	1.00	46.59		C
ATOM	2360	CG	TYR	Α	436	66.196	55.715	-0.312	1.00	47.13		C
ATOM	2361	CD1	TYR	Α	436	65.599	54.485	-0.585	1.00	47.53		C
MOTA	2362	CD2	TYR	Α	436	65.713	56.843	-0.974	1.00	47.79		С
ATOM	2363	CE1	TYR	Α	436	64.547	54.380	-1.493	1.00	48.14	•	С
MOTA	2364	CE2	TYR	Α	436	64.661	56.751	-1.882	1.00	48.43		С
ATOM	2365	CZ	TYR	A	436	64.083	55.517	-2.136	1.00	48.48		C
MOTA	2366	OH	TYR	Α	436	63.036	55.424	-3.024	1.00	49.29		0
MOTA	2367	N	VAL	Α	437	68.786	54.412	3.140	1.00	41.44		N
ATOM	2368	CA	VAL	Α	437	70.018	54.251	3.901	1.00	39.25		C
ATOM	2369	C			437	70.997	53.500	3.010		37.73		С
ATOM	2370	0			437	70.604	52.608	2.261		37.14	•	. 0
ATOM	2371	СВ			437	69.786	53.455	5.209		38.97		С
ATOM	2372		VAL			68.841	54.225	6.119		39.50		С
ATOM	2373		VAL			69.221	52.084	4.901		38.52		C
ATOM	2374	N			438	72.289	53.852	3.075		37.00		N
ATOM	2375	CA			438	73.280	53.169	2.239		35.94		C
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ATOM	2376	С	PRO	A	438	•	73.390	51.682	2.547	1.00 3	4.96		С
MOTA	2377	0	PRO	Α	438		73.442	51.282	3.710	1.00 3	4.43		0
ATOM	2378	CB	PRO	Α	438		74.569	53.929	2.543	1.00 3	6.50		C
ATOM	2379	CG	PRO	Α	438		74.377	54.345	3.981	1.00 3	7.42		С
ATOM	2380	CD	PRO	A	438		72.935	54.813	3.988	1.00 3	7.02		C
MOTA	2381	N	TYR	Α	439		73.412	50.872	1.492	1.00 3			N
MOTA	2382	CA	TYR	Α	439		73.526	49.423	1.619	1.00 3	2.47		C
MOTA	2383	C	TYR	Α	439		74.858	49.089	2.284	1.00 3			C
ATOM	2384	0	TYR	A	439		75.881	49.681	1.959	1.00 3			0
ATOM	2385	CB	TYR	Α	439		73.459	48.778	0.232	1.00 3			C
MOTA	2386	CG	TYR	Α	439		73.590	47.273	0.230	1.00 3			C
MOTA	2387	CD1	TYR	Α	439		72.683	46.476	0.925	1.00 3			C
ATOM	2388	CD2	TYR	Α	439		74.601	46.643	-0.497	1.00 3			C
MOTA	2389	CE1	TYR				72.775	45.087	0.896	1.00 3			C
ATOM	2390	CE2	TYR				74.702	45.254	-0.533	1.00 3			C
ATOM	2391	CZ			439		73.784	44.484	0.165	1.00 3			C
MOTA	2392	OH	TYR				73.863	43.112	0.124	1.00 3			0
ATOM	2393	N	ALA				74.847	48.133	3.208	1.00 3			N
MOTA	2394	CA	ALA				76.070	47.765	3.913	1.00 3			C
ATOM	2395	C	ALA				76.429	46.297	3.758	1.00 3			C
ATOM	2396	0	ALA				77.465	45.856	4.244	1.00 3			0
ATOM	2397	CB	ALA				75.938	48.115	5.396	1.00 3			C
ATOM	2398	N	GLY				75.577	45.538	3.080	1.00 3			N
ATOM	2399	CA	GLY				75.857	44.127	2.899	1.00 3			C
ATOM	2400	C	GLY				75.250	43.262	3.991	1.00 3			C
ATOM	2401	0	GLY				74.248	43.639	4.602	1.00 3			
ATOM	2402	N	LYS				75.867	42.106	4.231	1.00 3			O
ATOM	2403	CA	LYS				75.411	41.147	5.235	1.00 3			N C
ATOM	2404	C	LYS				75.531	41.671	6.664	1.00 3			
MOTA	2405	0	LYS				76.495	42.350	7.012	1.00 3			C
ATOM	2406	CB	LYS				76.216	39.848	5.129	1.00 3			0
ATOM	2407	CG	LYS				76.072	39.097	3.814	1.00 3			C
ATOM	2408	CD	LYS				74.734	38.377	3.714	1.00 3			C
ATOM	2409	CE	LYS				74.725	37.415	2.527	1.00 4			C
ATOM	2410	NZ	LYS				73.453	36.640	2.425	1.00 4			C
ATOM	2411	N	LEU				74.548	41.332	7.491	1.00 4			N
ATOM	2412	CA	LEU				74.538	41.751	8.887	1.00 3			N
ATOM	2413	C	LEU				75.790	41.271	9.624	1.00 2			C
ATOM	2414	Ö	LEU				76.430	42.040	10.343	1.00 2			C
ATOM	2415	CB	LEU				73.281	41.208	9.582				0
ATOM	2416	CG	LEU				73.124	41.454	11.087	1.00 28			C
ATOM	2417		LEU			•	71.648	41.409	11.471	1.00 2			C
ATOM	2418		LEU				73.920	40.408					C
ATOM	2419	N	LYS				76.136	40.408	11.863	1.00 28			C
ATOM	2420	CA	LYS				77.282	39.382	9.423 10.083	1.00 29			N
ATOM	2421	C	LYS				78.583	40.179		1.00 30			C
ATOM	2422	0	LYS			`	79.124		10.103	1.00 30			С
ATOM	2423	CB	LYS				77.562	40.453	11.174	1.00 30			0
ATOM	2424	CG	LYS					38.002	9.477	1.00 3			C .
ATOM	2425	CD	LYS				78.712	37.262	10.164	1.00 34			C
ATOM	2426	CE	LYS				78.908 80.016	35.868	9.587	1.00 36			C
ATOM	2427	NZ	LYS					35.126	10.314	1.00 3			C
ATOM	2427		ASP				81.325	35.828	10.197	1.00 38			N
ATOM	2429		ASP				79.087	40.542	8.927	1.00 30			N
ATOM	2429		ASP				80.344	41.280	8.829	1.00 33			C
ATOM	2430		ASP				80.303	42.662	9.462	1.00 30			С
ATOM	2431		ASP			•	81.296	43.125	10.022	1.00 29			0
111 OF	4734	CD	MOP	A	<del>4</del> 43		80.757	41.412	7.363	1.00 33	3.63		С

MOTA	2433	CG	ASP	A	445	80.781	40.079	6.650	1.00 35.	59		С
MOTA	2434	QD1	ASP	A	445	81.474	39.158	7.136	1.00 36.	48		0
MOTA	2435	OD2	ASP	Α	445	80.102	39.953	5.610	1.00 37.	36		0
MOTA	2436	N			446	79.157	43.321	9.366	1.00 28.	50		N
MOTA	2437	CA			446	79.005	44.657	9.922	1.00 28.	18		С
MOTA	2438	C	ASN	A	446	78.957	44.660	11.450	1.00 27.	76		С
MOTA	2439	0	ASN	Α	446	79.575	45.506	12.092	1.00 27.	57		0
MOTA	2440	CB			446	77.750	45.306	9.347	1.00 28.	54		C
ATOM	2441	CG			446	77.938	45.755	7.909	1.00 28.	71		C
ATOM	2442		ASN			78.508	46.815	7.652	1.00 29.	33		0
MOTA	2443	ND2	ASN			77.473	44.945	6.967	1.00 27.	37		N
MOTA	2444	N			447	78.222	43.714	12.023	1.00 27.3	34		N
MOTA	2445	CA			447	78.105	43.600	13.474	1.00 27.	57		C
ATOM	2446	C			447	79.461	43.220	14.071	1.00 28.3	37		C
MOTA	2447	0			447	79.878	43.770	15.088	1.00 28.4	12		0
MOTA	2448	CB			447	77.043	42.542	13.850	1.00 27.3	28		C
MOTA	2449		VAL			77.154	42.172	15.324	1.00 26.0	57		C
MOTA	2450	CG2	VAL	Α	447	75.657	43.091	13.553	1.00 26.5	56		C
MOTA	2451	N	GLU	Α	448	80.151	42.287	13.426	1.00 28.8	39		N
ATOM	2452	CA	GLU	Α	448	81.464	41.861	13.897	1.00 30.0	)4		C
MOTA	2453	C	GLU			82.412	43.061	13.971	1.00 29.3	L3		C
MOTA	2454	0	GLU			83.127	43.239	14.960	1.00 28.3	39		0
MOTA	2455	CB	GLU	A	448	82.029	40.790	12.959	1.00 32.2	21		C
MOTA	2456	CG	GLU			83.451	40.343	13.273	1.00 35.9	95		C
MOTA	2457	CD	GLU			83.912	39.210	12.365	1.00 38.4	16		C
MOTA	2458	OE1	GLU	Α	448	83.834	39.364	11.124	1.00 40.3	L <b>4</b>		0
MOTA	2459	OE2				84.351	38.163	12.890	1.00 40.4	1		0
ATOM	2460	N	ALA			82.404	43.889	12.930	1.00 27.9	90		N
MOTA	2461	CA	ALA			83.265	45.069	12.893	1.00 27.6			C
MOTA	2462	C	ALA			82.870	46.080	13.974	1.00 27.2	21		C
MOTA	2463	0	ALA			83.725	46.612	14.685	1.00 26.6	8		0
ATOM	2464	CB	ALA			83.203	45.722	11.513	1.00 28.3			C
ATOM	2465	N	SER			81.573	46.343	14.097	1.00 26.1	.7		N
ATOM	2466	CA	SER			81.090	47.279	15.105	1.00 26.5	52		C
ATOM	2467	C	SER			81.487	46.829	16.511	1.00 26.5			C
ATOM	2468	0	SER			82.062	47.603	17.281	1.00 26.6			0
ATOM	2469	CB	SER			79.562	47.408	15.032	1.00 26.1			C
ATOM .	2470	OG	SER			79.154	48.048	13.833	1.00 25.9			0
ATOM	2471	N	LEU			81.186	45.575	16.839	1.00 25.7			N
ATOM	2472	CA	LEU			81.490	45.045	18.163	1.00 26.0		٠.	С
ATOM	2473	C	LEU			82.986	44.910	18.450	1.00 26.5			С
MOTA MOTA	2474	0	LEU			83.404	44.961	19.611	1.00 25.9			0
ATOM	2475 2476	CB	LEU			80.767	43.709	18.372	1.00 25.3			C
ATOM		CG	LEU			79.238	43.840	18.305	1.00 25.0			C
ATOM	2477		LEU			78.586	42.524	18.693	1.00 24.9			C
ATOM	2478 2479	N	LEU ASN			78.773	44.962	19.232	1.00 25.2			C
ATOM	2479	CA	ASN			83.796	44.747	17.407	1.00 26.9		•	N
ATOM	2480	C	ASN			85.240	44.661 46.016	17.618	1.00 28.1			C
ATOM	2482	0	ASN			85.722		18.133	1.00 27.5			C
ATOM	2482	CB	ASN			86.624 85.977	46.094	18.968	1.00 26.7			0
ATOM	2483	CG	ASN			85.977 86.089	44.310	16.320	1.00 30.2			C
ATOM	2485		ASN			86.089 86.244	42.815	16.099	1.00 33.7			C
ATOM	2486		ASN			86.034	42.048 42.393	17.050	1.00 36.5			0
ATOM	2487	ND2	LYS			85.104	42.393	14.839 17.632	1.00 35.3			N
ATOM	2488	CA	LYS			85.453	48.435	18.043	1.00 27.2 1.00 27.3			N
ATOM	2489	C	LYS			84.962	48.684					C
		•				04.304	40.004	19.465	1.00 26.3	د		C

MOTA	2490	0	LYS	A	453		85.654	49.305	20.267	1.00 25.7	4	0
MOTA	2491	CB	LYS	Α	453		84.835	49.453	17.076	1.00 29.1	8	C
MOTA	2492	CG	LYS	A	453		85.374	49.322	15.651	1.00 31.5	7	C
ATOM	2493	CD	LYS	A	453		84.545	50.103	14.637	1.00 33.4	3 .	C
MOTA	2494	CE	LYS	A	453		84.630	51.604	14.856	1.00 34.7	9 .	C
ATOM	2495	NZ	LYS	Α	453		83.781	52.334	13.861	1.00 35.7	8	N
MOTA	2496	N			454		83.764	48.197	19.772	1.00 25.1		N
ATOM	2497	CA			454		83.200	48.351	21.104	1.00 24.1	8	C
ATOM	2498	C			454		84.108	47.638	22.114	1.00 24.7	7	C
MOTA	2499	0			454		84.455	48.194	23.159	1.00 23.5		0
ATOM	2500	CB			454		81.770	47.741	21.180	1.00 24.4		С
ATOM	2501		VAL				81.293	47.691	22.627	1.00 23.6		C
ATOM	2502		VAL				80.800	48.574	20.338	1.00 23.7		С
ATOM	2503	N			455		84.501	46.409	21.791	1.00 24.4		N
ATOM	2504	CA			455		85.355	45.634	22.683	1.00 24.9		С
MOTA	2505	C			455		86.728	46.266	22.878	1.00 25.1		C
ATOM	2506	0			455		87.273	46.254	23.984	1.00 24.4		0
MOTA	2507	CB			455		85.477	44.194	22.168	1.00 25.6		C .
ATOM ATOM	2508	CG			455		84.136	43.465	22.213	1.00 27.1		C
ATOM	2509 2510	CD CE			455		84.249	41.968	21.985	1.00 28.5		C
ATOM	2511	NZ			455 455		84.339	41.611	20.517	1.00 29.6		C
ATOM	2512	N			456	-	84.059 87.282	40.156	20.315	1.00 30.7		N
ATOM	2512	CA			456		88.583	47.478	21.810 21.895	1.00 24.8		N
ATOM	2514	C			456		88.477	48.690	22.831	1.00 26.0 1.00 25.4		C
ATOM	2515	o			456		89.337	48.908	23.689	1.00 25.4		C
ATOM	2516	CB			456		89.046	47.920	20.501	1.00 23.0		0 C
ATOM	2517	OG			456		90.355	48.454	20.559	1.00 27.0		0
ATOM	2518	N			457		87.414	49.471	22.671	1.00 30.8		· N
ATOM	2519	CA			457		87.214	50.640	23.520	1.00 24.2		C
ATOM	2520	C			457	-	86.999	50.197	24.968	1.00 23.7		C
ATOM	2521	Ō			457	•	87.484	50.835	25.900	1.00 23.1		0
ATOM	2522	CB			457		86.013	51.470	23.035	1.00 24.6		Č
ATOM	2523	OG1			457		86.268	51.918	21.699	1.00 25.5		Ö
ATOM	2524	CG2	THR			•	85.791	52.680	23.934	1.00 24.5		Ċ
ATOM	2525	N	MET	Α	458		86.285	49.092	25.155			N
ATOM	2526	CA	MET	Α	458		86.054	48.582	26.500	1.00 23.6		C
MOTA	2527	C	MET	Α	458		87.395	48.265	27.160	1.00 23.6		C
MOTA	2528	.0	MET	Α	458		87.582	48.522	28.351	1.00 23.5		0
ATOM	2529	СВ	MET	Α	458		85.157	47.339	26.453	1.00 22.3		С
ATOM	2530	CG	MET	Α	458		83.680	47.680	26.256	1.00 22.5		С
MOTA	2531	SD	MET	Α	458		82.608	46.247	26.043	1.00 23.3	2	· s
ATOM	2532	CE	MET				82.688	45.515	27.705	1.00 22.3	2 .	C
MOTA	2533	N	CYS				88.332	47.716	26.393	1.00 24.0	5	N
ATOM	2534	CA	CYS				89.649	47.413	26.947	1.00 25.5	6	C
MOTA	2535	C	CYS	А	459		90.409	48.701	27.281	1.00 25.1	3	C
ATOM	2536	0	CYS				91.214	48.725	28.215	1.00 24.6	1	0
ATOM	2537	CB	CYS				90.465	46.548	25.985	1.00 28.4	9	C
ATOM	2538	SG	CYS				90.054	44.772	26.089	1.00 33.4	0	S
ATOM	2539	N	ASN				90.160	49.766	26.519	1.00 24.0		N
ATOM	2540	CA	ASN				90.804	51.047	26.793	1.00 24.3		С
ATOM	2541	C	ASN				90.302	51.515	28.155	1.00 24.0		С
MOTA	2542	0	ASN				91.029	52.148	28.915	1.00 23.2		0
ATOM	2543	CB	ASN				90.412	52.110	25.759	1.00 24.6		C
ATOM	2544	CG	ASN				91.081	51.909	24.415	1.00 25.7		C
ATOM	2545		ASN				90.405	51.787	23.399	1.00 27.0		0
MOTA	2546	ממו	ASN	А	460		92.410	51.889	24.399	1.00 24.4	6	N

ATOM	2547	N	CYS	A	461	89.042	51.205	28.448	1.00	23.87		N
ATOM	2548	CA	CYS	Α	461	88.422	51.611	29.704	1.00	24.41		С
ATOM	2549	С	CYS			88.660	50.633	30.848	1.00	24.32		С
ATOM	2550	0			461	88.180	50.852	31.958	1.00	25.56		0
ATOM	2551	CB			461	86.918	51.806	29.496		24.60		C
ATOM	2552	SG	CYS			86.525	53.116	28.308		26.96		S
ATOM	2553	N			462	89.389	49.556	30.570		24.32		N
ATOM	2554	CA	GLY			89.685	48.558	31.587		24.60		C
ATOM	2555	C			462	88.547	47.600	31.907		25.06		C
ATOM	2556	0	GLY			88.465	47.076	33.024		24.53		Ö
ATOM	2557	N	ALA			87.682	47.343	30.929		24.46		N
ATOM	2558	CA			463	86.539	46.463	31.147		24.56		C
ATOM	2559	C			463	86.489	45.254	30.234		24.52		C
ATOM	2560	0	ALA			86.647	45.372	29.018		24.90		0
ATOM	2561	СВ	ALA			85.246	47.257	31.000		24.47		C
ATOM	2562	N			464	86.246	44.092	30.834		24.58	,	N
ATOM	2563	CA			464	86.139	42.840	30.096		24.71		C
ATOM	2564		LEU			84.683	42.423	29.927		23.91		C
ATOM	2565	0			464	84.387	41.458	29.224		24.47		0
ATOM	2566	CB	LEU				41.720	30.823		25.91	*	C
ATOM	2567	CG	LEU			86.887 88.397	41.720	30.623		27.36		C
			LEU									C
ATOM	2568 2569		LEU			88.947	40.476 41.420	31.448		28.44		C
ATOM ATOM		N			465	88.702		29.147		27.33		
	2570					83.782	43.131	30.596		22.92		N
ATOM	2571	CA			465	82.354	42.831	30.512		22.25		C
ATOM	2572	C			465	81.568	44.129	30.548		21.44		C
ATOM	2573	0			465	82.104	45.177	30.891		20.34	_	0
ATOM	2574	CB			465	81.862	41.981	31.699		22.45		C
ATOM	2575	OG1			465	81.932	42.762	32.899		22.22		0
ATOM	2576	CG2	THR			82.710	40.726	31.858		22.79		C
ATOM	2577	N			466	80.288	44.052	30.214		21.19		N
ATOM	2578	CA			466	79.447	45.236	30.230		20.76		C
ATOM	2579	C			466	79.254	45.736	31.666		20.40		C
ATOM	2580	0			466	79.358	46.929	31.927		19.90		0
ATOM	2581	CB			466	78.098	44.944	29.530		21.19		C
ATOM	2582		ILE			78.356	44.780	28.022		21.38		C
ATOM	2583		ILE			77.100	46.073	29.792		21.25		C
ATOM	2584	CD1	ILE			77.152	44.290	27.219		22.58		C
ATOM	2585	N			467	78.995		32.626				N
ATOM	2586	CA			467	78.822	45.333	33.991				C
ATOM	2587	C			467	80.094	46.009	34.510		21.02	·	C
ATOM	2588	0			467	80.025	47.006	35.216		21.23		0
ATOM	2589	CB			467	78.461	44.076	34.782		20.94		C
ATOM	2590	CG			467	77.717	43.250	33.750		20.39		C
ATOM	2591	CD			467	78.606	43.411	32.538		19.76		C
ATOM	2592	N			468	81.259	45.475	34.160		21.22		N
MOTA	2593	CA			468	82.491	46.093	34.627		21.96		. C
MOTA	2594	C			468	82.648	47.477	33.992		22.09		C
	. 2595	0			468	83.108	48.412	34.644		22.10		0
ATOM	2596	CB			468	83.709	45.217	34.308		22.23		C
ATOM	2597	CG			468	85.015	45.839	34.780		22.84		C
ATOM	2598	CD			468	86.211	44.908	34.692		22.48		C
ATOM	2599		GLN			86.355	44.141	33.740		22.48		0
ATOM	2600		GLN			87.097	44.997	35.683		22.38		N
ATOM	2601	N			469	82.264	47.603	32.722		21.64		N
ATOM	2602	CA			469	82.344	48.886	32.027		21.89		C
· ATOM	2603	C .	LEU	Α	469	81.434	49.905	32.714	1.00	22.01		С

MOTA	2604	0	LEU	Α	469	81.818	51.051	32.925	1.00 21.53		0
MOTA	2605	CB.	LEU	Α	469	81.904	48.735	30.564	1.00 21.51		С
MOTA	2606	CG			469	81.761	50.027	29.745	1.00 22.03		С
ATOM	2607		LEU			83.134	50.627	29.484	1.00 21.95		С
ATOM	2608		LEU			81.056	49.727	28.414	1.00 22.12		C
ATOM	2609	N			470	80.225	49.473	33.058	1.00 22.00		N
											C
MOTA	2610	CA			470	79.254	50.349	33.696	1.00 23.44		
ATOM	2611	C	GLN			79.743	50.838	35.055	1.00 24.51		C
MOTA	2612	0			470	79.377	51.922	35.513	1.00 25.02		0
MOTA	2613	CB			470	77.917	49.612	33.817	1.00 23.09		C
ATOM	2614	CG			470	77.402	49.156	32.439	1.00 23.12		С
MOTA	2615	CD	GLN	Α	470	76.092	48.397	32.492	1.00 22.83		C
MOTA	2616	OE1	GLN	Α	470	75.855	47.613	33.406	1.00 23.32		0
ATOM	2617	NE2	$\operatorname{GLN}$	Α	470	75.242	48.610	31.488	1.00 21.97		N
ATOM	2618	N	SER	Α	471	80.590	50.039	35.687	1.00 25.04		N
MOTA	2619	CA	SER	Α	471	81.139	50.391	36.983	1.00 26.85		С
ATOM	2620	C			471	82.378	51.284	36.863	1.00 27.29		С
ATOM	2621	Ō			471 .	82.530	52.246	37.614	1.00 27.87		Ō
ATOM	.2622	CB			471	81.500	49.115	37.749	1.00 27.07		C
	2623	OG				82.193	49.422	38.943	1.00 30.83		0
ATOM					471				•		
ATOM	2624	N			472	83.244	50.981	35.900	1.00 27.53		N
ATOM	2625	CA			472	84.496	51.723	35.732	1.00 28.78		C
ATOM	2626	C			472	84.519	52.903	34.768	1.00 27.72		C
MOTA	2627	0			472	85.421	53.733	34.840	1.00 27.66		0
ATOM	2628	CB	LYS	Α	472	85.604	50.752	35.316	1.00 29.70		C
MOTA	2629	ÇG	LYS	Α	472	85.789	49.598	36.274	1.00 33.23		С
ATOM	2630	CD	LYS	Α	472	86.819	48.602	35.768	1.00 33.84.		С
ATOM	2631	CE	LYS	Α	472	88.218	49.184	35.759	1.00 34.76		C
MOTA	2632	NZ	LYS	A	472	89.209	48.107	35.470	1.00 34.52		N
ATOM	2633	N			473	83.548	52.976	33.865	1.00 26.96		N
ATOM	2634	CA			473	83.522	54.045	32.870	1.00 26.73		C
ATOM	2635	C			473	83.663	55.472	33.395	1.00 26.34		C
ATOM	2636	0			473	83.045	55.853	34.389	1.00 26.04		0
MOTA	2637	CB			473	82.250	53.936	32.023	1.00 26.80		C
							56.248		1.00 26.28		N
ATOM	2638	N			474	84.502		32.713		•	
ATOM	2639	CA			474	84.712	57.656	33.034	1.00 26.69		C
ATOM	2640	C .			474	84.166	58.376	31.807	1.00 26.49		C
ATOM	2641	0			474	84.724	58.278	30.712	1.00 25.96		0
MOTA	2642	CB			474	86.202	57.955	33.241	1.00 27.26		C
ATOM	2643	CG :	LYS			86.777	57.279	34.485	$1.00\ 28.54$		C
MOTA	2644	CD	LYS	Α	474	88.207	57.724	34.778	1.00 30.16		С
MOTA	2645	CE	LYS	A	474	89.177	57.220	33.745	1.00 30.74		С
MOTA	2646	NZ	LYS	Α	474	90.571	57.651	34.057	1.00 30.36		N
ATOM	2647	N	ILE	Α	475	83.067	59.095	31.995	1.00 26.72		N
MOTA	2648	CA	ILE	A	475	82.403	59.763	30.885	1.00 27.59	•	С
ATOM	2649	С			475	82.413	61.281	30.960	1.00 28.14		С
MOTA	2650	0			475	81.900	61.871	31.910	1.00 28.29		0
ATOM	2651	СВ			475	80.943	59.278	30.794	1.00 27.25		C
ATOM	2652				475	80.919	57.743	30.797	1.00 27.67		Ċ
ATOM	2653				475	80.281	59.832	29.537	1.00 27.73		C
						•					С
MOTA	2654				475	79.522	57.134	30.885	1.00 26.56		
ATOM	2655	N			476	82.982	61.912	29.941	1.00 28.53	e • *	N
ATOM	2656	CA			476	83.045	63.364	29.916	1.00 29.40		C
ATOM	2657	C				82.184	63.974	28.820	1.00 29.85		C
ATOM	2658	0				82.029	63.407	27.734	1.00 28.69		0
MOTA	2659	CB			476		63.865	29.722	1.00 29.27		С
MOTA	2660	OG1	THR	A	476	84.501	65.293	29.813	1.00 30.19		0

ATOM	2661	CG2	THR	A	476	85.027	63.445	28.353	1.00 28	.75	-	С
MOTA	2662	N	LEU	Α	477	81.615	65.133	29.126	1.00 30	. 92		N
MOTA	2663	CA	LEU	Α	477	80.791	65.863	28.176	1.00 33			С
ATOM	2664	С			477		66.681	27.363	1.00 34			c
ATOM	2665	0			477	82.829	67.084	27.887	1.00 34			0
ATOM	2666	СВ			477	79.831	66.795	28.925	1.00 34			C
ATOM	2667	CG			477	78.671						
							67.452	28.173	1.00 35			C
ATOM	2668		LEU			77.683	66.393	27.716	1.00 34			С
ATOM	2669		LEU			77.975	68.449	29.094	1.00 35			C
ATOM	2670	N			478	81.497	66.910	26.089	1.00 36			N
MOTA	2671	CA			478	82.388	67.688	25.234	1.00 37	.55		С
MOTA	2672	C	VAL	A	478	81.741	69.041	24.929	1.00 38	.64		С
MOTA	2673	0	VAL	A	478	80.517	69.151	24.884	1.00 37	.96		0
MOTA	2674	CB	VAL	A	478	82.681	66.929	23.919	1.00 37	.92		С
MOTA	2675	CG1	VAL	Α	478	83.612	67.732	23.046	1.00 38	.33		С
ATOM	2676	CG2	VAL	A	478	83.308	65.577	24.234	1.00 38	.01		С
MOTA	2677	N	SER	Α	479	82.559	7.0.073	24.733	1.00 40			N
ATOM	2678	CA			479	82.034	71.408	24.452	1.00 42			C
MOTA	2679	C			479	81.414	71.483	23.062	1.00 43			C
ATOM	2680	Ö			479	81.868	70.818	22.130	1.00 43			
ATOM	2681		SER									0
MOTA						83.139	72.465	24.572	1.00 41			C
	2682	OG			479	84.069	72.363	23.508	1.00 41			0
ATOM	2683	N			480	80.373	72.299	22.930	1.00 45			N
ATOM	2684	CA			480	79.688 ⁻	72.465	21.653	1.00 48			С
ATOM	2685	C			480	80.615	73.067	20.602	1.00 49	.80		С
MOTA	2686	0	SER	A	480	80.426	72.859	19.402	1.00 50	.06		0
ATOM	2687	CB	SER	Α	480	78.450	73.352	21.830	1.00 48	.66		С
MOTA	2688	OG	SER	Α	480	78.778	74.574	22.468	1.00 50	.04		0
ATOM	2689	N	VAL	A	481	81.622	73.805	21.062	1.00 51	.44		N
ATOM	2690	CA	VAL	A	481	82.584	74.442	20.168	1.00 53			С
MOTA	2691	С	VAL			83.452	73.408	19.462	1.00 53			C
ATOM	2692	0	VAL			83.755	73.544	18.277	1.00 54			ō
ATOM	2693	CB	VAL			83.515	75.402	20.936	1.00 53			C
ATOM	2694	CG1				84.397	76.161	19.958	1.00 53			C
ATOM	2695		VAL			82.698	76.363					C
ATOM	2696	N			482		70.303	21.775 20.199	1.00 53			
						83.858			1.00 55			N
ATOM	2697	CA	SER			84.695	71.324	19.642	1.00 56			C
ATOM	2698	C	SER			83.890	70.412	18.722	1.00 57			С
ATOM	2699	0	SER			84.454	69.577	18.012	1.00 57		,	0
ATOM	2700	CB	SER			85.319	70.499	20.767	1.00 56	.17		C
MOTA	2701	OG	SER			84.315	69.924		1.00 56	.14	٠.	0
MOTA	2702	N	ILÉ			82.571	70.572	18.742	1.00 57	.97		N
MOTA	2703	CA	ILE	А	483	81.693	69.769	17.899	1.00 58	.92		С
MOTA	2704	C	ILE	Α	483	81.319	70.545	16.639	1.00 59	.33		С
MOTA	2705	0	ILE	Α	483	81.588	70.028	15.535	1.00 59	.84		0
MOTA	2706	CB	ILE	Α	483	80.399	69.375	18.645	1.00 59	.00		С
ATOM	2707	CG1	ILE	Α	483	80.744	68.544	19.883	1.00 59			С
MOTA	2708	CG2	ILE	Α	483	79.485	68.585	17.716	1.00 59			Ċ
ATOM	2709		ILE			79.543	68.155	20.718	1.00 59			Ċ
TER	2710		ILE					20.720	1.00 33	• - '		_
HETATM		K			900	52.243	59.799	29.172	0.75 29	54	•	v
HETATM		P	IMP	7-1								K
					602	67.273	54.643	14.906	1.00 25			P
HETATM		01P			602	66.861	54.580	13.478	1.00 26			0
HETATM		02P			602	68.037	53.408	15.254	1.00 26			0
HETATM		.03P			602	68.090	55.908	15.218	1.00 25			0
HETATM		05*			602	66.048	54.751	15.914	1.00 25			0
HETATM	2717	C5*	IMP		602	65.054	53.735	15.819	1.00 23	.90		C

HETATM	2718	C4*	IMP	602	63.955	53.909	16.822	1.00 23.17	С
HETATM	2719	04*	IMP	602	63.226	55.091	16.335	1.00 22.32	0
HETATM	2720	C3 *	IMP	602	62.855	52.875	16.958	1.00 22.53	C
HETATM	2721	03*	IMP	602	63.229	51.710	17.687	1.00 21.85	ō
HETATM	2722	C2*	IMP	602	61.776	53.670	17.629	1.00 22.98	C
HETATM		02*	IMP	602	61.948	53.736	19.029	1.00 22.76	0
HETATM		C1*	IMP	602	61.928	55.030	16.924	1.00 23.55	. C
HETATM		N9	IMP	602	60.928	55.202	15.816	1.00 24.16	N
HETATM		C8	IMP	602	60.310	54.298	14.971	1.00 25.51	C
HETATM		N7	IMP	602	59.490	54.866	14.137	1.00 25.31	N
HETATM		C5	IMP	602	59.548	56.197	14.417	1.00 25.42	C
HETATM		C6	IMP	602	58.866	57.320	13.831	1.00 25.42	C
HETATM		06	IMP	602	58.049	57.320	12.909	1.00 20.39	. 0
HETATM		N1	IMP	602	59.213	58.576	14.425	1.00 27.34	
HETATM		C2	IMP	602	60.131	58.702	15.478	1.00 26.89	N
HETATM		N3	IMP	602	60.765				C
HETATM		C4	IMP			57.630	16.021	1.00 25.55	N
HETATM		C1		602	60.437	56.438	15.458	1.00 25.01	C
HETATM			MOA	600	59.312	58.341	19.371	1.00 30.41	C
HETATM		C2	MOA	600	54.700	56.341	16.455	1.00 32.49	C
		C3	MOA	600	53.578	55.627	16.198	1.00 33.53	C
HETATM		C4	AOM	600	52.262	56.261	16.628	1.00 34.60	C
HETATM		C5	MOA	600	51.704	55.529	17.856	1.00 35.56	C
HETATM		C6	AOM	600	52.413	55.880	19,153		C
HETATM		C7	MOA	600	58.717	53.456	19.827	1.00 29.24	C
HETATM		C8	AOM	600	55.639	53.144	18.309	1.00 29.52	C
HETATM		C9	AOM	600	53.564	54.254	15.513	1.00 33.79	· C
HETATM			MOA	600	59.889	56.364	20.539	1.00 29.78	C
HETATM			AOM	600	58.905	56.011	19.445	1.00 29.43	C
HETATM			AOM	600	58.347	54.721	19.086	1.00 29.74	С
HETATM			MOA	600	57.416	54.689	17.974	1.00 30.13	C
HETATM			AOM	600	57.077	55.910	17.275	1.00 30.94	C
HETATM			AOM	600	57.655	57.164	17.672	1.00 30.68	C
HETATM		C16	MOA	600	58.569	57.183	18.763	1.00 30.24	Ċ
HETATM		C17	MOA	600	56.107	55.881	16.099	1.00 32.03	C
HETATM		01	MOA	600	59.306	59.497	19.082	1.00 30.18	0
HETATM	2753	02	MOA	600	60.036	57.818	20.365	1.00 29.58	0
HETATM	2754	03	MOA	600	56.876	53.479	17.608	1.00 30.38	0
HETATM	2755	04	MOA	600	57.314	58.318	16.987	1.00 32.33	0
HETATM	2756	05	MOA	600	52.401	57.074	19.536	1.00 37.48	0
HETATM	2757	06	MOA.	600	52.985	54.959	19.780	1.00 35.87	0
HETATM	2758	0 1	HOH	1	59.924	29.679	22.414	1.00 50.51	0
HETATM	2759	0	HOH	2	79.013	41.426	29.423	1.00 18.90	0.
HETATM	2760	0	HOH	3	58.751	44.934	36.922	1.00 19.77	0
HETATM	2761	0	HOH	4	70.195	53.954	21.764	1.00 22.57	0
HETATM	2762	0	HOH	5	65.251	60.127	24.411	1.00 21.78	0
METATM	2763	0	HOH	6	75.493	43.370	30.924	1.00 20.48	0
HETATM	2764	0	HOH	7	56.253	78.397	34.291	1.00 25.40	0
HETATM	2765	0	HOH	. 8		47.704	38.822	1.00 22.86	. 0
HETATM	2766	0	HOH	9	56.894	58.199	28.230	1.00 22.26	0.
HETATM	2767	0	нон	10	70.506	52.801	14.222	1.00 25.03	Ō
HETATM	2768	0	нон	11	63.871	40.741	7.794	1.00 24.61	Ō
HETATM	2769	0	нон	12	60.616	40.963	2.773	1.00 57.79	0
HETATM		0	нон	13	72.961 -		35.993	1.00 22.52	0
HETATM		0	НОН	14	74.407	45.323	32.761	1.00 26.87	0
HETATM		Ō	нон	15	86.443	54.944	31.105	1.00 24.24	0
HETATM		0	нон	16	64.957	58.145	21.206	1.00 24.24	0
HETATM		0	нон	17	58.226	37.978	34.604	1.00 28.06	0
	, •	-		<u>.</u> ,	50.220	5570	54.004	1.00 20.00	J

HETATM	2775	0	HOH	18	65.737	37.023	16.608	1.00 23.81	0
HETATM	2776	0	HOH	19	71.973	37.555	33.842	1.00 27.82	0
HETATM	2777	0	HOH	20	61.772	38.247	34.046	1.00 22.62	0
HETATM	2778	0	HOH	21	52.301	52.152	19.306	1.00 49.95	0
HETATM	2779	0	HOH	22	87.828	53.279	33.165	1.00 28.88	0
HETATM	2780	0	нон	23	81.359	62.610	21.058	1.00 27.37	0
HETATM		0	нон	24	75.817	40.774	32.087	1.00 26.13	0
HETATM		0	нон	25	58.057	34.952	27.087	1.00 28.97	ō
HETATM		0	нон	26	83.688	52.415	20.816	1.00 30.28	ō
HETATM		0	нон	27	77.149	53.162	34.368	1.00 29.69	ō
HETATM	•	0	нон	28	56.074	56.906	38.662	1.00 37.23	o
HETATM		Ō	НОН	29	49.870	31.480	16.451	1.00 33.88	0
HETATM		0	НОН	30	73.925	34.558	39.925	1.00 28.68	0
HETATM		Ō	нон	31	78.589	39.852	31.836	1.00 26.69	0
HETATM		Ö	НОН	32	59.193	50.825	9.635	1.00 20.03	0
HETATM		0	НОН	33	48.757	43.664	20.942	1.00 30.46	0
HETATM		Ö	нон	34	63.470	55.921	20.034	1.00 23.40	0
HETATM		0	нон	35	64.748	36.350	34.843	1.00 20.43	0
HETATM		0	нон	36	74.476	38.378	31.025	1.00 29.99	0
HETATM		0	нон	37	51.517	53.493	25.810	1.00 30.13	
HETATM		0	НОН	38	67.426				0
HETATM		0	НОН	39	73.458	38.071	46.103	1.00 30.22	0
HETATM		0.	нон НОН			50.410	36.144	1.00 28.96	0
HETATM		0		40	48.967	53.101	24.116	1.00 49.76	0
HETATM			HOH	41	70.826	32.483	29.970	1.00 39.88	0
		0	HOH	42	61.107	50.022	17.672	1.00 23.40	0
HETATM		0	нон	43	73.974	36.418	10.780	1.00 31.43	0
HETATM		0	НОН	44	50.211	45.778	35.694	1.00 31.02	0
HETATM		0	НОН	45	63.973	35.222	38.133	1.00 49.08	0
HETATM		0	нон	46	52.459	51.210	38.008	1.00 33.23	0
HETATM		0	HOH	47	68.639	62.467	21.428	1.00 33.95	0
HETATM		0	нон	48	69.432	33.097	27.354	1.00 32.47	0
HETATM		0	нон	49	74.578	37.941	8.159	1.00 32.47	0
HETATM		0	НОН	50	58.916	51.450	16.416	1.00 29.63	0
HETATM		0	НОН	51	69.598	53.385	17.586	1.00 29.79	0
HETATM		0	HOH	52	47.572	53.766	36.762	1.00 39.69	0
HETATM		0	HOH	53	84.793	48.751	39.168	1.00 43.51	0
HETATM		0	НОН	54.	59.544	49.841	20.045	1.00 33.31	0
HETATM		0	НОН	55	64.161	25.507	14.641	1.00 30.60	0
HETATM		0	HOH	56	55.066	70.757	16.127	1.00 32.83	0
HETATM		0	НОН	57	74.182	47.486	35.548	1.00 31.59	0
HETATM		0	HOH	58	62.583	34.645	41.460	1.00 39.46	0
HETATM		0	нон	59	51.561	30.405	13.105	1.00 57.09	0
HETATM		0	HOH	60	47.880	31.075	25.095	1.00 39.60	0
HETATM		0	HOH	61	53.997	32.961	37.361	1.00 38.91	0
HETATM		0	HOH	62	84.739	38.545	32.721	1.00 34.80	0
HETATM		0	HOH	63	70.499	56.677	14.512	1.00 31.54	0
HETATM		0	HOH	64	96.766	42.780	26.087	1.00 48.54	0
HETATM		0	HOH	65	48.178	56.536	26.666	1.00 44.06	0
HETATM		0	нон	66	55.822	40.800	37.347	1.00 41.31	0
HETATM		0	HOH	67 .	62.651	58.499	18.259	1.00 30.38	0
HETATM		0	HOH	68	78.584	37.867	17.336	1.00 35.48	0
HETATM		0	HOH	69	73.741	59.595	37.699	1.00 46.66	0
HETATM		Ο.	HOH	70	61.930	61.268	37.149	1.00 35.16	0
HETATM		0	HOH	71	64.600	31.307	29.524	1.00 40.08	0
HETATM		0	HOH	72	68.630	35.309	7.689	1.00 35.28	0
HETATM		0	HOH	73	74.821	69.567	31.440	1.00 45.20	0
HETATM	2831	0	HOH	74	60.851	32.866	26.981	1.00 36.07	0

HETATM	2832	0	HOH	75	78.209	47.346	37.269	1.00 42.78		0
HETATM	2833	0	HOH	76	78.477	34.764	30.567	1.00 40.04		0
HETATM	2834	0	HOH	77	71.498	30.722	23.744	1.00 35.11		Ō
HETATM	2835	0	НОН	78	64.709	27.584	26.706	1.00 39.53		Ö
HETATM		0	нон	79	58.218	44.875	5.808	1.00 39.15		0
HETATM		0	нон	80	91.925	40.314	20.235	1.00 47.22		0
HETATM		0	нон	81	65.374	28.271	14.859	1.00 33.66		0
HETATM		Ō	НОН	82	86.254	46.969	13.548	1.00 33.00		0
HETATM		Ō	НОН	83	86.599	66.411	30.817	1.00 42.03		0
HETATM		Ö	нон	84	62.054	33.096		1.00 28.32		0
HETATM		0	нон	85	95.032	45.638	27.312	1.00 43.30		
HETATM		0	нон	86	50.747	50.260				0
HETATM		0	нон	87			21.915	1.00 33.76		0
HETATM		0	нон		64.754	61.086	37.994	1.00 43.01		0
HETATM		0	HOH	88 89	70.920	55.587	41.621	1.00 30.53		0
HETATM		0			87.356	35.892	30.913	1.00 54.42		0
HETATM			HOH	90	58.062	50.894	22.714	1.00 36.70		0
		0	НОН	91	66.375	33.870	36.838	1.00 36.70		0
HETATM		0	нон	92	80.489	54.081	12.959	1.00 34.92		0
HETATM		.0	HOH	93	49.688	32.577	11.671	1.00 44.86	•	0
HETATM		0	нон	94	59.901	34.059	37.276	1.00 46.67		Ō
HETATM		0	НОН	. 95	60.124	37.261	37.104	1.00 40.44		0
HETATM		0	НОН	96	68.062	43.325	0.440	1.00 40.55		0
HETATM		0	НОН	97	92.043	48.470	23.328	1.00 41.20		0
HETATM		0	HOH	98	91.696	47.559	34.606	1.00 36.60		0
HETATM		0	нон	99	72.456	40.842	41.613	1.00 38.50		0
HETATM		0	HOH	100	56.000	31.198	23.572	1.00 40.79		0
HETATM		0	нон	101	49.154	42.288	7.689	1.00 40.98		0
HETATM		0	нон	102	73.470	34.115	8.839	1.00 54.10		0
HETATM		0	HOH	103	61.679	22.463	5.705	1.00 52.66		0
HETATM	2861	0	HOH	104	77.579	33.064	16.137	1.00 47.51		0
HETATM	2862	0	HOH	105	44.253	34.815	19.536	1.00 42.37		0
HETATM		0	HOH	106	45.451	48.437	27.057	1.00 38.64		0
HETATM	2864	0	HOH	107	59.592	41.005	40.036	1.00 41.25		0
HETATM	2865	0	HOH	108	72.057	60.543	20.606	1.00 36.69		0
HETATM	2866	0	HOH	109	55.706	47.432	14.991	1.00 42.24		0
HETATM	2867	0	HOH	110	62.531	31.016	25.446	1.00 42.66		0
HETATM	2868	0	HOH	111	73.718	48.291	39.771	1.00 53.04		0
HETATM	2869	0	HOH	112	83.522	36.024	30.729	1.00 43.33		0
HETATM	2870	O	НОН	113	45.028	41.039	12.802	1.00 37.34		0
HETATM	2871	0	нон	114	69.524	61.101				0
HETATM	2872	0	нон	115	44.452	44.556	32.827	1.00 42.61		Ō
HETATM	2873	0	HOH	116	54.399	50.470	15.469	1.00 48.43		Ō
HETATM	2874	0	нон	117	61.680	63.886	35.352	1.00 38.29		Ö
HETATM	2875	0	нон	118	77.475	37.083	32.225	1.00 42.79		Ö
HETATM		0	НОН	119	53.086	57.730	38.200	1.00 44.72		0
HETATM		0	нон	120 `	79.877	44.361	4.154	1.00 44.06		o
HETATM		0	нон	121	57.773	49.349	44.295	1.00 43.42		0
HETATM		0	НОН	122	81.021	37.925	24.041	1.00 40.18		0
HETATM		0	нон	123	. 92.237	46.682	19.335	1.00 49.83		0
HETATM		0	НОН	124	80.220	47.967	11.064	1.00 40.72		0
HETATM		Ö	нон	125	73.280	38.459	40.030	1.00 40.72		0
HETATM		Ö	нон	126	75.038	35.191	27.031	1.00 48.03		0
HETATM		Ö	нон	127	54.075	73.213	39.117	1.00 50.72		
HETATM		0	нон	128	53.079	51.663	12.707	1.00 36.72	•	0
HETATM		0	нон	129	60.212	50.703	45.884			
HETATM		0	нон	130	85.493	38.286	29.721	1.00 49.07 1.00 45.03		0
HETATM		0	НОН	131	72.246	32.952				0
	2000	•	поп	+J +	12.240	34.734	26.073	1.00 44.35		0

HETATM	2889	0	HOH	132	74.333	61.925	18.775	1.00 48.91	0
HETATM	2890	0	HOH	133	78.475	36.361	24.540	1.00 37.31	0
HETATM	2891	0	нон	134	70.535	25.345	24.416	1.00 53.34	0
HETATM	2892	0	нон	135	81.081	38.943	20.640	1.00 56.12	0
HETATM	2893	0	HOH	136 .	60.987	73.452	38.941	1.00 44.96	0
HETATM	2894	0	нон	137	72.007	45.634	46.667	1.00 47.04	0
HETATM		0	нон	138	54.881	54.255	40.087	1.00 47.22	0
HETATM		Ō	НОН	139	64.127	73.162	32.500	1.00 39.03	0
HETATM		Ō	НОН	140	91.015	51.135	35.563	1.00 54.84	0
HETATM		Ō	НОН	141	44.237	42.950	15.139	1.00 48.61	o
HETATM		0	нон	142	84.958	38.682	22.430	1.00 41.83	. 0
HETATM		0	нон	143	58.380	41.590	5.816	1.00 48.19	0
HETATM		0	нон	144	83.941	42.401	9.407	1.00 45.78	0
HETATM		0	нон	145	48.035	32.860	14.382	1.00 49.29	. 0
HETATM		0	нон	146					
HETATM		0			62.470	25.629	24.500	1.00 47.15	0
HETATM		-	HOH	147	65.188	30.631	26.633	1.00 37.87	0
		0	HOH	148	77.128	50.319	38.016	1.00 50.84	0
HETATM		0	нон	149	42.757	43.332	23.225	1.00 33.93	0
HETATM		0	НОН	150	58.953	59.302	30.126	1.00 39.39	0
HETATM		0	НОН	151 .	55.806	76.784	37.029	1.00 43.89	0
HETATM		0	нон	152	90.603	36.990	30.793	1.00 49.14	0
HETATM		0	НОН	153 ·	73.243	28.912	13.776	1.00 44.78	0
HETATM		0	нон	154	67.670	43.878	49.116	1.00 67.50	0
HETATM		0	HOH	155	65.834	40.753	2.745	1.00 47.30	0
HETATM		0	HOH .	156	73.843	26.459	21.225	1.00 51.06	0
HETATM		0	нон	157	47.543	41.292	37.139	1.00 43.81	0
HETATM		0	HOH	158	68.949	44.995	46.463	1.00 50.27	0
HETATM	2916	0	HOH	159	65.492	48.526	5.504	1.00 49.51	. 0
HETATM	2917	0	HOH	160	61.797	59.722	40.006	1.00 48.68	. 0
HETATM	2918	0	HOH	161	55.273	30.697	8.635	1.00 52.97	0
HETATM	2919	0	HOH	162	50.769	46.331	39.662	1.00 54.24	0
HETATM	2920	0	HOH ·	163	55.705	37.312	5.362	1.00 48.34	0
HETATM	2921	0	HOH	164	71.788	35.831	6.649	1.00 44.94	0
HETATM	2922	0	нон	165	56.757	27.304	17.057	1.00 47.57	0
HETATM	2923	0	нон	166	65.426	40.295	46.540	1.00 43.83	Ō
HETATM		0	нон	167	55.456	40.561	4.913	1.00 53.90	0
HETATM		0	нон	168	66.954	59.058	38.463	1.00 50.46	. 0
HETATM		0	нон	169	71.615	66.882	31.700	1.00 48.78	ō
HETATM		0	нон	170	73.024	64.238	30.477	1.00 52.09	ō
HETATM		0	нон	171			51.024		. 0
HETATM		o	нон	172			6.859		0
HETATM		Ö	НОН	173			-4.830		0
HETATM		Ö	нон	174		49.280		1.00 53.36	0
HETATM		0	нон	175		53.016		1.00 53.20	0
HETATM		0	нон	176		71.708	31.475		
HETATM		0	НОН	177	71.233			1.00 48.45	0
HETATM		0	НОН	178		53.697	43.927	1.00 52.05	. 0
HETATM						64.308	17.573	1.00 54.16	. 0
		0	НОН		89.336	53.769	35.871	1.00 53.70	0
HETATM		0.	НОН	180	54.353	46.276	17.782	1.00 54.59	0
HETATM		0	НОН	181	68.022	31.001	25.937	1.00 44.50	0
HETATM		0	HOH	182	52.980	29.445	10.465	1.00 50.22	0
HETATM		0	НОН	183	56.686	28.215	9.903	1.00 56.33	0
HETATM		0	НОН	184		49.876	10.573	1.00 53.98	0
HETATM		0	НОН	185		49.900	11.756	1.00 57.59	0
HETATM		0	НОН	186		47.021	8.192	1.00 51.32	0
HETATM		0	НОН		76.430	51.542			0
HETATM	2945	0	НОН	188	75.167	53.201	-1.226	1.00 44.07	0

TABLE 3 180

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HETATM 2946 O HOH 189
                               62.348 54.827 1.013 1.00 51.43
HETATM 2947 O HOH 190 59.995 64.398 17.439 1.00 60.65
HETATM 2948 O HOH 191 97.267 51.029 39.970 1.00 58.50
HETATM 2949 O HOH 192 97.537 47.953 39.149 1.00 64.57
HETATM 2950 O HOH 193 93.132 47.026 37.250 1.00 46.96
CONECT 202 2538
CONECT 1536 1537
CONECT 1537 1536 1538 1540
CONECT 1538 1537 1539
CONECT 1539 1538 1542
CONECT 1540 1537 1541
CONECT 1541 1540
CONECT 1542 1539
CONECT 2538 202
CONECT 2712 2713 2714 2715 2716
CONECT 2713 2712 .
CONECT 2714 2712
CONECT 2715 2712
CONECT 2716 2712 2717
CONECT 2717 2716 2718
CONECT 2718 2717 2719 2720
CONECT 2719 2718 2724
CONECT 2720 2718 2721 2722
CONECT 2721 2720
CONECT 2722 2720 2723 2724
CONECT 2723 2722
CONECT 2724 2719 2722 2725
CONECT 2725 2724 2726 2734
CONECT 2726 2725 2727
CONECT 2727 2726 2728
CONECT 2728 2727 2729 2734
CONECT 2729 2728 2730 2731
CONECT 2730 2729
CONECT 2731 2729 2732
CONECT 2732 2731 2733
CONECT 2733 2732 2734
CONECT 2734 2725 2728 2733
CONECT 2735 2750 2752 2753
CONECT 2736 2737 2751
CONECT 2737 2736 2738 2743
CONECT 2738 2737 2739
CONECT 2739 2738 2740
CONECT 2740 2739 2756 2757
CONECT 2741 2746
CONECT 2742 2754
CONECT 2743 2737
CONECT 2744 2745 2753
CONECT 2745 2744 2746 2750
CONECT 2746 2741 2745 2747
CONECT 2747 2746 2748 2754
CONECT 2748 2747 2749 2751
CONECT 2749 2748 2750 2755
CONECT 2750 2735 2745 2749
CONECT 2751 2736 2748
CONECT 2752 2735 .
CONECT 2753 2735 2744
CONECT 2754 2742 2747
```

0

0

TABLE 3 181

CONECT 2755 2749 CONECT 2756 2740 CONECT 2757 2740

MASTER 520 0 4 14 18 0 0 6 2949 1 55 39

END .

Figure 12 P-UC 5440 Page 69

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62 TABLE 3

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HEADER OXIDOREDUCTASE
                                              08-AUG-02
                                                         1MEI
        INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
TITLE
        2 TRITRICHOMONAS FOETUS WITH XMP AND MYCOPHENOLIC ACID BOUND
TITLE
COMPND MOL ID: 1;
COMPND 2 MOLECULE: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE;
COMPND 3 CHAIN: A:
COMPND 4 SYNONYM: IMP DEHYDROGENASE, IMPDH:
COMPND 5 EC: 1.1.1.205;
COMPND 6 ENGINEERED: YES
SOURCE
       MOL ID: 1;
SOURCE
        2 ORGANISM SCIENTIFIC: TRITRICHOMONAS FOETUS;
SOURCE 3 GENE: IMPDH;
SOURCE 4 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE 5 EXPRESSION SYSTEM COMMON: BACTERIA;
SOURCE 6 EXPRESSION_SYSTEM_STRAIN: H712;
SOURCE 7 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE 8 EXPRESSION_SYSTEM_PLASMID: PBACE.
KEYWDS ALPHA BETA BARREL
EXPDTA X-RAY DIFFRACTION
AUTHOR G.L.PROSISE, H.LUECKE
JRNL
       AUTH G.L.PROSISE, H.LUECKE
JRNL
         TITL CRYSTAL STRUCTURE OF T. FOETUS INOSINE
        TITL 2 MONOPHOSPHATE DEHYDROGENASE IN COMPLEX WITH
JRNL
JRNL
         TITL 3 SUBSTRATE, COFACTOR, AND ANALOGS:STRUCTURAL BASIS
        TITL 4 FOR THE RANDOM-IN ORDERED-OUT KINETIC MECHANISM
JRNL
         REF
JRNL
                 TO BE PUBLISHED
         REFN
JRNL
REMARK 1
REMARK 2
REMARK 2 RESOLUTION. 2.20 ANGSTROMS.
REMARK 3
REMARK
        3 REFINEMENT.
REMARK 3 PROGRAM
                      : CNS 1.1
REMARK 3
          AUTHORS
                      : BRUNGER, ADAMS, CLORE, DELANO, GROS, GROSSE-
REMARK 3
                      : KUNSTLEVE, JIANG, KUSZEWSKI, NILGES, PANNU,
REMARK 3
                      : READ, RICE, SIMONSON, WARREN
REMARK 3
REMARK 3 REFINEMENT TARGET : ENGH & HUBER
REMARK 3
REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.20
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 33.06
REMARK 3 DATA CUTOFF
                                (SIGMA(F)) : 0.000
REMARK 3 OUTLIER CUTOFF HIGH (RMS(ABS(F))) : NULL
REMARK 3 COMPLETENESS (WORKING+TEST) (%): 99.5
REMARK 3 NUMBER OF REFLECTIONS
                                          : 32648
REMARK 3
REMARK
        3 FIT TO DATA USED IN REFINEMENT.
                                         : THROUGHOUT
REMARK 3 CROSS-VALIDATION METHOD
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING SET): 0.227
REMARK 3 FREE R VALUE
                                         : 0.257
REMARK 3 FREE R VALUE TEST SET SIZE (%): 5.200
REMARK 3 FREE R VALUE TEST SET COUNT : 1709
REMARK 3 ESTIMATED ERROR OF FREE R VALUE : 0.006
REMARK 3
REMARK
      3 FIT IN THE HIGHEST RESOLUTION BIN.
```

```
REMARK 3 TOTAL NUMBER OF BINS USED
         3 TOTAL NUMBER OF BINS USED : 6
3 BIN RESOLUTION RANGE HIGH (A): 2.20
3 BIN RESOLUTION RANGE LOW (A): 2.34
 REMARK
 REMARK
 REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 96.60
 REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 4936
REMARK 3 BIN R VALUE
                                 (WORKING SET) : 0.2710
 REMARK 3 BIN FREE R VALUE
 REMARK 3 BIN FREE R VALUE TEST SET SIZE (%): 5.00
 REMARK 3 BIN FREE R VALUE TEST SET COUNT : 259
 REMARK 3
             ESTIMATED ERROR OF BIN FREE R VALUE : 0.018
 REMARK 3
 REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
 REMARK 3 PROTEIN ATOMS : 2690
 REMARK 3 NUCLEIC ACID ATOMS
                                    : 0
REMARK 3 HETEROGEN ATOMS : 48
REMARK 3 SOLVENT ATOMS : 186
                                    : 180
 REMARK 3
 REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : 27.40
 REMARK 3 MEAN B VALUE (OVERALL, A**2): 37.30
 REMARK 3 OVERALL ANISOTROPIC B VALUE.
 REMARK 3 B11 (A**2) : 0.00000
 REMARK 3 B22 (A**2) : 0.00000
 REMARK 3 B33 (A**2) : 0.00000
 REMARK 3
           B12 (A**2) : 0.00000
 REMARK 3
           B13 (A**2) : 0.00000
 REMARK 3 B23 (A**2) : 0.00000
REMARK 3
 REMARK 3 ESTIMATED COORDINATE ERROR.
 REMARK 3 ESD FROM LUZZATI PLOT (A): 0.27
 REMARK 3 ESD FROM SIGMAA
                                       (A) : 0.23
 REMARK 3 LOW RESOLUTION CUTOFF
                                        (A) : 5.00
REMARK 3
 REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
 REMARK 3 ESD FROM C-V LUZZATI PLOT (A): 0.32
 REMARK 3 ESD FROM C-V SIGMAA
                                        (A) : 0.28
 REMARK 3
 REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS (DECE
                                        (A) : 0.006
REMARK 3 BOND ANGLES (DEGREES) : 1.20
REMARK 3 DIHEDRAL ANGLES (DEGREES) : 22.50
REMARK 3 IMPROPER ANGLES (DEGREES) : 0.68
REMARK 3
 REMARK 3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                                 RMS SIGMA
REMARK 3 MAIN-CHAIN BOND (A**2): 1.230; 1.500
REMARK 3 MAIN-CHAIN ANGLE (A**2): 2.190; 2.000
REMARK 3 SIDE-CHAIN BOND (A**2): 1.610; 2.000
REMARK 3
REMARK 3
           SIDE-CHAIN ANGLE
                                        (A**2) : 2.520 ; 2.500
REMARK 3
REMARK 3 BULK SOLVENT MODELING.
REMARK 3 METHOD USED : FLAT MODEL
REMARK 3 KSOL : 0.34
                       : 35.45
REMARK 3 BSOL
REMARK 3
REMARK 3 NCS MODEL : NULL
```

```
REMARK 3
REMARK 3 NCS RESTRAINTS.
           MCS RESTRAINTS.

GROUP 1 POSITIONAL

GROUP 1 B-FACTOR

(A): NULL; NULL

(A**2): NULL; NULL
                                                  RMS SIGMA/WEIGHT
REMARK 3
REMARK 3
REMARK 3
REMARK 3 PARAMETER FILE 1 : PROTEIN REP.PARAM
REMARK 3 PARAMETER FILE 2 : PARAM.GNSOL
REMARK 3 PARAMETER FILE 3 : CIS PEPTIDE.PARAM
REMARK 3 PARAMETER FILE 4 : MPA.PAR
REMARK 3 PARAMETER FILE 5 : XMP.PAR
REMARK 3 PARAMETER FILE 6 : NULL
REMARK 3 TOPOLOGY FILE 1 : PROTEIN.TOP
REMARK 3 TOPOLOGY FILE 2 : XMP.TOP
REMARK 3 TOPOLOGY FILE 3 : MPA.TOP
REMARK 3 TOPOLOGY FILE 4 : K.TOP
REMARK 3 TOPOLOGY FILE 5 : TOPH.GNSOL
REMARK 3 TOPOLOGY FILE 6 : NULL
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: NULL
REMARK 4
REMARK 4 1MEI COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 16-AUG-2002.
REMARK 100 THE RCSB ID CODE IS RCSB016853.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION REMARK 200 DATE OF DATA COLLECTION : 11-APR-2001
REMARK 200 EXPERIMENT TYPE
REMARK 200 TEMPERATURE (KELVIN) : 100.0
                                       : 7.50
REMARK 200 PH
REMARK 200 NUMBER OF CRYSTALS USED
                                          : 1
REMARK 200
REMARK 200 RADIATION SOURCE : SS
REMARK 200 BEAMLINE : O
                                   : SSRL
                                        : 9-1
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A) : 0.97
REMARK 200 MONOCHROMATOR
                                        : NULL
REMARK 200 OPTICS
                                         : NULL
REMARK 200
REMARK 200 DETECTOR TYPE
                                       : IMAGE PLATE
REMARK 200 DETECTOR TYPE : IMAGE PLATE REMARK 200 DETECTOR MANUFACTURER : MARRESEARCH
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE
                                   : SCALEPACK
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 32815
REMARK 200 RESOLUTION RANGE HIGH (A): 2.200 REMARK 200 RESOLUTION RANGE LOW (A): 99.00
                                     (A): 99.000
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NULL
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE (%): 99.5
REMARK 200 DATA REDUNDANCY
                                      : 4.700
REMARK 200 R MERGE
                                     (I) : 0.06600
REMARK 200 R SYM
                                     (I) : NULL
REMARK 200 <I/SIGMA(I) > FOR THE DATA SET : 21.4000
```

```
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A): 2.20
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.24
REMARK 200 COMPLETENESS FOR SHELL (%): 98.7
REMARK 200 DATA REDUNDANCY IN SHELL : NULL
REMARK 200 R MERGE FOR SHELL (I) : 0.50000
REMARK 200 R SYM FOR SHELL
                                    (I) : NULL
REMARK 200 <1/SIGMA(1) > FOR SHELL
                                        : 2.900
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: FOURIER SYNTHESIS
REMARK 200 SOFTWARE USED: CNS
REMARK 200 STARTING MODEL: PDB ENTRY 1AK5
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: SODIUM MALONATE, TRIS, 2-
REMARK 280 MERCAPTOETHANOL, EDTA, GLYCEROL
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 4 3 2
REMARK 290
REMARK 290
              SYMOP SYMMETRY
REMARK 290
             NNNMMM OPERATOR
REMARK 290
              1555
                      X,Y,Z
REMARK 290
               2555
                      -X,-Y,Z
              3555
REMARK 290
                      -X,Y,-Z
              4555 X,-Y,-Z
REMARK 290
REMARK 290 5555 Z, X, Y
REMARK 290 6555 Z, -X, -Y
REMARK 290 7555 -Z, -X, Y
REMARK 290
              8555 -Z,X,-Y
              9555 Y,Z,X
REMARK 290
          10555 -Y,Z,-X
11555 Y,-Z,-X
REMARK 290
REMARK 290
REMARK 290 12555 -Y,-Z,X
REMARK 290
              13555 Y, X, -Z
REMARK 290 14555 -Y,-X,-Z
REMARK 290
             15555 Y,-X,Z
REMARK 290
             16555 -Y,X,Z
REMARK 290
              17555 X,Z,-Y
REMARK 290
              18555
                      -X,Z,Y
             19555
REMARK 290
                      -X,-Z,-Y
REMARK 290
              20555 X,-Z,Y
REMARK 290
              21555 Z,Y,-X
REMARK 290
             22555 Z,-Y,X
REMARK 290
             23555 -Z,Y,X
             24555 -Z,-Y,-X
REMARK 290
REMARK 290
REMARK 290 WHERE NNN -> OPERATOR NUMBER
REMARK 290
                  MMM -> TRANSLATION VECTOR
REMARK 290
```

REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY REMARK 290 RELATED MOLECULES. SMTRY1 1 1.000000 0.000000 0.000000 0.00000 REMARK 290 REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.00000 REMARK 290 2 -1.000000 0.000000 0.000000 SMTRY1 0.00000 REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 3 -1.000000 0.000000 0.000000 0.00000 REMARK 290 3 0.000000 1.000000 0.000000 0.00000 SMTRY2 REMARK 290 SMTRY3 3 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY1 4 1.000000 0.000000 0.000000 0.00000 REMARK 290 4 0.000000 -1.000000 0.000000 0.00000 SMTRY2 4 0.000000 0.000000 -1.000000 REMARK 290 SMTRY3 0.00000 5 0.000000 0.000000 1.000000 REMARK 290 SMTRY1 0.00000 REMARK 290 SMTRY2 5 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 5 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY1 6 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY2 6 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 6 0.000000 -1.000000 0.000000 0.00000 REMARK 290 7 0.000000 0.000000 -1.000000 SMTRY1 0.00000 7 -1.000000 0.000000 0.000000 REMARK 290 SMTRY2 0.00000 7 0.000000 1.000000 0.000000 REMARK 290 SMTRY3 0.00000 8 0.000000 0.000000 -1.000000 REMARK 290 SMTRY1 0.00000 REMARK 290 SMTRY2 8 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 8 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY1 9 0.000000 1.000000 0.000000 0.00000 REMARK 290 9 0.000000 0.000000 1.000000 SMTRY2 0.00000 SMTRY3 9 1.000000 0.000000 0.000000 REMARK 290 0.00000 SMTRY1 10 0.000000 -1.000000 0.000000 REMARK 290 0.00000 REMARK 290 SMTRY2 10 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY3 10 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 11 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 11 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY3 11 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 12 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 12 0.000000 0.000000 -1.000000 0.00000 REMARK 290 12. 1.000000 0.000000 0.000000 SMTRY3 0.00000 REMARK 290 SMTRY1 13 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 13 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 13 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY1 14 0.000000 -1.000000 0.000000 0.00000 . 0.00000 SMTRY2 14 -1.000000 0.000000 0.000000 REMARK 290 REMARK 290 SMTRY3 14 0.000000 0.000000 -1.000000 0.00000 SMTRY1 15 0.000000 1.000000 0.000000 REMARK 290 0.00000 SMTRY2 15 -1.000000 0.000000 0.000000 REMARK 290 0.00000 REMARK 290 SMTRY3 15 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 16 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 16 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 16 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 17 1.000000 0.000000 0.000000 0.00000 SMTRY2 17 0.000000 0.000000 1.000000 REMARK 290 0.00000 SMTRY3 17 0.000000 -1.000000 0.000000 REMARK 290 0.00000 SMTRY1 18 -1.000000 0.000000 0.000000 REMARK 290 0.00000 REMARK 290 SMTRY2 18 0.000000 0.000000 1.000000 0.00000

```
REMARK 290 SMTRY3 18 0.000000 1.000000 0.000000
                                                             0.00000
           SMTRY1 19 -1.000000 0.000000 0.000000
REMARK 290
                                                              0.00000
           SMTRY2 19 0.000000 0.000000 -1.000000
                                                         0.00000
REMARK 290
REMARK 290 SMTRY3 19 0.000000 -1.000000 0.000000
                                                             0.00000
REMARK 290 SMTRY1 20 1.000000 0.000000 0.000000
                                                              0.00000
REMARK 290 SMTRY2 20 0.000000 0.000000 -1.000000
REMARK 290 SMTRY3 20 0.000000 1.000000 0.000000
                                                             0.00000
REMARK 290 SMTRY1 21 0.000000 0.000000 1.000000
                                                             0.00000
REMARK 290 SMTRY2 21 0.000000 1.000000 0.000000 REMARK 290 SMTRY3 21 -1.000000 0.000000 0.000000 REMARK 290 SMTRY1 22 0.000000 0.000000 1.000000 REMARK 290 SMTRY1 22 0.000000 0.000000 1.000000
                                                             0.00000
                                                             0.00000
                                                             0.00000
REMARK 290 SMTRY2 22 0.000000 -1.000000 0.000000
                                                             0.00000
REMARK 290 SMTRY3 22 1.000000 0.000000 0.000000
                                                             0.00000
REMARK 290 SMTRY1 23 0.000000 0.000000 -1.000000
                                                             0.00000
REMARK 290 SMTRY2 23 0.000000 1.000000 0.000000
                                                           0.00000
           SMTRY3 23 1.000000 0.000000 0.000000
REMARK 290
                                                             0.00000
REMARK 290 SMTRY1 24 0.000000 0.000000 -1.000000 REMARK 290 SMTRY2 24 0.000000 -1.000000 0.000000
                                                              0.00000
                                                             0.00000
REMARK 290 SMTRY3 24 -1.000000 0.000000 0.000000
                                                             0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 1 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000
                                                             0.00000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000
                                                              0.00000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000 REMARK 350 BIOMT1 2 -1.000000 0.000000 0.000000 REMARK 350 BIOMT2 2 0.000000 -1.000000 0.000000
                                                             0.00000
                                                            155.07000
                                                            155.07000
REMARK 350 BIOMT3 2 0.000000 0.000000 1.000000
                                                             0.00000
REMARK 350 BIOMT1 3 0.000000 1.000000 0.000000
                                                              0.00000
REMARK 350 BIOMT2 3 -1.000000 0.000000 0.000000
                                                            155.07000
REMARK 350 BIOMT3 3 0.000000 0.000000 1.000000
                                                             0.00000
REMARK 350 BIOMT1 4 0.000000 -1.000000 0.000000
                                                            155.07000
REMARK 350 BIOMT2 4 1.000000 0.000000 0.000000
                                                             0.00000
           BIOMT3 4 0.000000 0.000000 1.000000
REMARK 350
                                                              0.00000
REMARK 375
REMARK 375 SPECIAL POSITION
REMARK 375 THE FOLLOWING ATOMS ARE FOUND TO BE WITHIN 0.15 ANGSTROMS
REMARK 375 OF A SYMMETRY RELATED ATOM AND ARE ASSUMED TO BE ON SPECIAL
REMARK 375 POSITIONS.
REMARK 375
REMARK 375 ATOM RES CSSEQI
REMARK 375
                HOH 131 LIES ON A SPECIAL POSITION.
REMARK 465
```

```
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465
              M RES C SSSEOI
REMARK 465
                MET A
                          1
REMARK 465
                GLY A
                        102
REMARK 465
                PHE A
                        103
REMARK 465
                VAL A
                        104
REMARK 465
                VAL A
                        105
REMARK 465
                SER A
                        106
REMARK 465
                ASP A
                        107
REMARK 465
                SER A
                        108
REMARK 465
                ASN A
                        109
REMARK 465
                VAL A
                        110
REMARK 465
                LYS A
                        111
REMARK 465
                PRO A
                        112
REMARK 465
                ASP A
                        113
REMARK 465
                GLN A
                        114
REMARK 465
                THR A
                        115
REMARK 465
                PHE A
                        116
REMARK 465
               ALA A
                        117
REMARK 465
                ASP A
                        118
REMARK 465
               VAL A
                        119
REMARK 465
               LEU A
                        120
REMARK 465
               ALA A
                        121
REMARK 465
                ILE A
                        122
REMARK 465
               SER A
                        123
REMARK 465
               GLN A
                        124
REMARK 465
               ARG A
                        125
REMARK 465
                THR A
                        126
REMARK 465
               THR A
                        127
REMARK 465
               HIS A
                        128
REMARK 465
               ASN A
                        129
REMARK 465
               THR A
                        130
REMARK 465
               VAL A
                        131
REMARK 465
               ALA A
                        132
REMARK 465
               VAL A
                        133
REMARK 465
               THR A
                        134
REMARK 465
               ASP A
                        135
REMARK 465
               ASP A
                        136
REMARK 465
               GLY A
                        137
REMARK 465
               THR A
                        138
REMARK 465
               PRO A
                        139
REMARK 465
               HIS A
                        140
REMARK 465
               GLY A
                        141
REMARK 465
               VAL A
                        142
REMARK 465
               LEU A
                        143
REMARK 465
               LEU A
                        144
REMARK 465
               GLY A
REMARK 465
               LEU A
                        146
REMARK 465
               VAL A
                        147
REMARK, 465
               THR A
                        148
REMARK 465
               GLN A
                        149
REMARK 465
               ARG A
                        150
REMARK 465
               ASP A
                        151
```

REMARK	465	TYR A	152
REMARK	465	PRO A	153
REMARK	465	ILE A	154
REMARK	465	ASP A	155
REMARK	465	LEU A	156
REMARK	465	THR A	157
REMARK	465	GLN A	158
REMARK	465	THR A	159
REMARK	465	GLU A	160
REMARK	465	THR A	161
REMARK	465	LYS A	162
REMARK	465	VAL A	163
REMARK	465	SER A	164
REMARK	465	ASP A	165
REMARK	465	MET A	166
REMARK	465	MET A	167
REMARK	465	THR A	168
REMARK	465	PRO A	169
REMARK	465	PHE A	170
REMARK	465	SER A	171
REMARK	465	LYS A	172
REMARK	465	LEU A	173
REMARK	465	VAL A	174
REMARK	465	THR A	175
REMARK	465	ALA A	176
REMARK	465	HIS A	177
REMARK	465	GLN A	178
REMARK	465	ASP A	179
REMARK	465	THR A	180
REMARK	465	LYS A	181
	465	LEU A	182
REMARK	465	SER A	183
REMARK	465	GLU A	184
REMARK	465	ALA A	185
REMARK	465	ASN A	186
	.465	LYS A	187
REMARK	465	ILE A	188
REMARK	465	ILE A	189
	465	TRP A	190
REMARK	465	GLU A	191
REMARK	465	LYS A	192
REMARK	465	LYS A	193
REMARK	465	LEU A	194
	465	ASN A	195
	465	ALA A	196
	465	LEU A	197
	465	PRO A	198
REMARK	465	ILE A	199
REMARK	465	ILE A	200
REMARK	465	ASP A	201
REMARK	465	ASP A	202
	465	ASP A	202
	465	GLN A	203
REMARK		HIS A	204
	465	LEU A	205
	465	ARG A	207
REMARK	465		
AMERICA	403	TYR A	208

```
REMARK 465
            ILE A 209
             VAL A
REMARK 465
                    210
             PHE A 211
REMARK 465
            ARG A 212
REMARK 465
          LYS A 213
REMARK 465
REMARK 465
            ASP A 214
REMARK 465
            TYR A 215
REMARK 465
            ASP A
                    216
           ARG A
REMARK 465
                    217
            SER A
REMARK 465
                    218
REMARK 465
          GLN A 219
REMARK 465
            VAL A 220
REMARK 465
            CYS A 221
REMARK 465
            GLN A 417
REMARK 465
            ARG A 418
REMARK 465
            TYR A 419
REMARK 465
             ASP A
                   420
REMARK 465
            LEU A
                   421
REMARK 465
           GLY A 422
REMARK 465
           GLY A 423
REMARK 465
            LYS A 424
REMARK 465
           GLN A 425
REMARK 465
            LYS A 426
            LEU A
                   427
REMARK 465
           VAL A
REMARK 465
                    484
REMARK 465
           GLU A 485
REMARK 465
           GLY A 486
REMARK 465
           GLY A 487
REMARK 465
           ALA A 488
REMARK 465
            HIS A 489
REMARK 465
            ASP A 490
                   491
REMARK 465
             VAL A
            ILE A
REMARK 465
                   492
            VAL A 493
REMARK 465
REMARK 465
           LYS A 494
REMARK 465
            ASP A 495
REMARK 465
            ARG A 496
REMARK 465
            ILE A 497
REMARK 465
            ASN A
                   498
REMARK 465
            ASP A
                    499
           TYR A
REMARK 465
                    500
REMARK 465
           HIS A 501
REMARK 465
            PRO A 502
REMARK 465
            LYS A
                    503
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI
REMARK 500 O GLY A 20 K
                                K A 900
                                                         2.12
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
```

```
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, 2 (A3, 1X, A1, I4, A1, 1X, A4, 3X), F6.3).
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1 RES CSSEQI ATM2
                                                       DEVIATION
                                    MET A 379 SD
REMARK 500
             MET A 379 CE
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1 ATM2
                                            ATM3
REMARK 500 ILE A 27 N - CA - C ANGL. DEV. = -7.8 DEGREES
                                 - CA - C ANGL. DEV. = -7.7 DEGREES
             GLN A 45 N
REMARK 500
REMARK 500 SER A 63 N - CA - C ANGL. DEV. = 8.3 DEGREES
REMARK 500 PHE A 266 N - CA - C ANGL. DEV. = -7.2 DEGREES REMARK 500 GLY A 312 N - CA - C ANGL. DEV. = 7.6 DEGREES
REMARK 500 GLY A 312 N - CA - C ANGL. DEV. = 7.6 DEGREES
REMARK 500 PRO A 391 N - CA - C ANGL. DEV. = 7.3 DEGREES
REMARK 500 LYS A 394 N - CA - C ANGL. DEV. = 7.3 DEGREES
REMARK 500 LYS A 472 N - CA - C ANGL. DEV. = -7.8 DEGREES
REMARK 500 LYS A 474 N - CA - C ANGL. DEV. = 8.3 DEGREES
REMARK 500 LYS A 474 N - CA - C ANGL. DEV. = -8.6 DEGREES
             LEU A 477 N - CA - C ANGL. DEV. = -7.6 DEGREES
REMARK 500
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: TORSION ANGLES
REMARK 500
REMARK 500 TORSION ANGLES OUTSIDE THE EXPECTED RAMACHANDRAN REGIONS:
REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 4X, F7.2, 3X, F7.2)
REMARK 500
REMARK 500 M RES CSSEQI
                                   PSI
                                               PHI
                              -106.74 -152.50
REMARK 500
              GLN A 324
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1AK5 RELATED DB: PDB
REMARK 900 INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
REMARK 900 TRITRICHOMONAS FOETUS
REMARK 900 RELATED ID: 1ME7
                                RELATED DB: PDB
REMARK 900 1ME7 CONTAINS THE SAME PROTEIN WITH RVP AND MOA BOUND
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REMARK 900 RELATED ID: 1ME8
                            RELATED DB: PDB
REMARK 900 1ME8 CONTAINS THE SAME PROTEIN WITH RVP BOUND
REMARK 900 RELATED ID: 1ME9 RELATED DB: PDB
REMARK 900 1ME9 CONTAINS THE SAME PROTEIN WITH IMP BOUND
REMARK 900 RELATED ID: 1MEH RELATED DB: PDB
REMARK 900 1MEH CONTAINS THE SAME PROTEIN WITH IMP AND MOA BOUND
REMARK 900 RELATED ID: 1MEW
                           RELATED DB: PDB
REMARK 900 1MEW CONTAINS THE SAME PROTEIN WITH XMP AND NAD BOUND
DBREF 1MEI A 1 503 SWS
                                        IMDH TRIFO
                               P50097
        1 A 503 MET ALA LYS TYR TYR ASN GLU PRO CYS HIS THR PHE ASN
SEORES
        2 A 503 GLU TYR LEU LEU ILE PRO GLY LEU SER THR VAL ASP CYS
SEORES
SEQRES
        3 A 503 ILE PRO SER ASN VAL ASN LEU SER THR PRO LEU VAL LYS
SEQRES
        4 A 503 PHE GLN LYS GLY GLN GLN SER GLU ILE ASN LEU LYS ILE
SEORES
       5 A 503 PRO LEU VAL SER ALA ILE MET GLN SER VAL SER GLY GLU
SEORES
       6 A 503 LYS MET ALA ILE ALA LEU ALA ARG GLU GLY GLY ILE SER
SEQRES
       7 A 503 PHE ILE PHE GLY SER GLN SER ILE GLU SER GLN ALA ALA
       8 A 503
SEQRES
                 MET VAL HIS ALA VAL LYS ASN PHE LYS ALA GLY PHE VAL
        9 A 503
SEQRES
                  VAL SER ASP SER ASN VAL LYS PRO ASP GLN THR PHE ALA
SEQRES 10 A 503 ASP VAL LEU ALA ILE SER GLN ARG THR THR HIS ASN THR
SEQRES 11 A 503 VAL ALA VAL THR ASP ASP GLY THR PRO HIS GLY VAL LEU
SEQRES 12 A 503 LEU GLY LEU VAL THR GLN ARG ASP TYR PRO ILE ASP LEU
SEORES 13 A 503
                 THR GLN THR GLU THR LYS VAL SER ASP MET MET THR PRO
SEQRES 14 A 503 PHE SER LYS LEU VAL THR ALA HIS GLN ASP THR LYS LEU
SEORES 15 A 503 SER GLU ALA ASN LYS ILE ILE TRP GLU LYS LYS LEU ASN
SEORES 16 A 503 ALA LEU PRO ILE ILE ASP ASP GLN HIS LEU ARG TYR
SEQRES 17 A 503
                 ILE VAL PHE ARG LYS ASP TYR ASP ARG SER GLN VAL CYS
SEQRES 18 A 503 HIS ASN GLU LEU VAL ASP SER GLN LYS ARG TYR LEU VAL
SEORES 19 A 503 GLY ALA GLY ILE ASN THR ARG ASP PHE ARG GLU ARG VAL
SEORES 20 A 503 PRO ALA LEU VAL GLU ALA GLY ALA ASP VAL LEU CYS ILE
SEQRES 21 A 503 ASP SER SER ASP GLY PHE SER GLU TRP GLN LYS ILE THR
SEQRES 22 A 503 ILE GLY TRP ILE ARG GLU LYS TYR GLY ASP LYS VAL LYS
SEQRES 23 A 503 VAL GLY ALA GLY ASN ILE VAL ASP GLY GLU GLY PHE ARG
SEQRES 24 A 503 TYR LEU ALA ASP ALA GLY ALA ASP PHE ILE LYS ILE GLY
SEQRES 25 A 503 ILE GLY GLY GLY SER ILE CYS ILE THR ARG GLU GLN LYS
SEQRES 26 A 503 GLY ILE GLY ARG GLY GLN ALA THR ALA VAL ILE ASP VAL
SEQRES 27 A 503 VAL ALA GLU ARG ASN LYS TYR PHE GLU GLU THR GLY ILE
SEQRES 28 A 503 TYR ILE PRO VAL CYS SER ASP GLY GLY ILE VAL TYR ASP
SEQRES 29 A 503 TYR HIS MET THR LEU ALA LEU ALA MET GLY ALA ASP PHE
SEQRES 30 A 503 ILE MET LEU GLY ARG TYR PHE ALA ARG PHE GLU GLU SER
SEQRES 31. A 503 PRO THR ARG LYS VAL THR ILE ASN GLY SER VAL MET LYS
SEQRES 32 A 503 GLU TYR TRP GLY GLU GLY SER SER ARG ALA ARG ASN TRP
SEQRES 33 A 503 GLN ARG TYR ASP LEU GLY GLY LYS GLN LYS LEU SER PHE
SEQRES 34 A 503 GLU GLU GLY VAL ASP SER TYR VAL PRO TYR ALA GLY LYS
SEQRES. 35 A 503 LEU LYS ASP ASN VAL GLU ALA SER LEU ASN LYS VAL LYS
SEQRES 36 A 503 SER THR MET CYS ASN CYS GLY ALA LEU THR ILE PRO GLN
       37 A 503 LEU GLN SER LYS ALA LYS ILE THR LEU VAL SER SER VAL
SEORES
       38 A 503 SER ILE VAL GLU GLY GLY ALA HIS ASP VAL ILE VAL LYS
SEQRES
      39 A 503
                  ASP ARG ILE ASN ASP TYR HIS PRO LYS
SEQRES
HET
        K A 900
                       1
HET
                      24
      XMP
            602
      MOA
HET
             600
                      23
HETNAM
            K POTASSIUM ION
HETNAM
          XMP XANTHOSINE-5'-MONOPHOSPHATE
HETNAM
          MOA MYCOPHENOLIC ACID
HETSYN
          XMP 5--MONOPHOSPHATE-9-BETA-D-RIBOFURANOSYL XANTHINE
HETSYN
          MOA 6-(1,3-DIHYDRO-7-HYDROXY-5-METHOXY-4-METHYL-1-
HETSYN
        2 MOA OXOISOBENZOFURAN-6-YL)-4-METHYL-4-HEXANOIC ACID
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FORMUL
            K
         2
                  K1 1+
FORMUL
         3 XMP
                 C10 H14 N4 O9 P1 1+
FORMUL
         4
           MOA
                 C17 H20 O6
FORMUL
         5 НОН
                *180(H2 O1)
HELIX
         1
           1 THR A
                      11 ASN A
                                 13
                                                                        3
HELIX
         2
           2 ILE A
                                 31 5
                      27
                         VAL A
                                                                        5
HELIX
         3
            3 GLY A
                      64 GLU A
                                 74 1
                                                                       11
HELIX
            4 SER A
         4
                     85
                         ASN A
                                 98
                                     1
                                                                       14
HELIX
         5
            5 ASP A 242
                          GLY A
                                254
                                     1
                                                                       13
             6 SER A
HELIX
         6
                    267
                          GLY A
                                 282
                                     1
                                                                       16
HELIX
         7
            7 ASP A 283
                         VAL A 285 5
                                                                       3
HELIX
         8
            8 ASP A 294
                         GLY A 305 1
                                                                       12
HELIX
         9
            9 GLY A
                    330
                         GLY A 350 1
                                                                       21
HELIX
        10
           10 TYR A 363 MET A 373 1
                                                                       11
HELIX
                         ARG A 386 1
        11 11 GLY A 381
                                                                       6
        12 12 SER A 410
HELIX
                          ASN A 415 1
                                                                       6
           13 LYS A 442
HELIX
        13
                          CYS A 461 1
                                                                       20
HELIX
        14
           14 THR A 465
                         ALA A 473 1
                                                                        9
SHEET
        1 A 2 TYR A 15 ILE A 18 0
SHEET
         2
           A 2 LYS A 474
                          LEU A 477 -1
                                        0
                                           LYS A 474
                                                         ILE A 18
                                                      N
SHEET
           B 2 THR A 35
        1
                          PRO A 36 0
           B 2 ASN A 49
SHEET
         2
                          LEU A 50 -1
                                        0
                                           LEU A 50
                                                      N
                                                         THR A 35
SHEET
            C 2 PHE A 40
                          GLN A 41 0
        1
SHEET
         2
            C 2 ILE A 351
                           TYR A 352 -1
                                        0
                                           TYR A 352
                                                      N
                                                         PHE A 40
SHEET
        1
            D 9 LEU A 54
                          SER A 56 0
SHEET
        2
            D 9 ILE A 77
                          ILE A 80 1
                                       0
                                           ILE A 77
                                                      N SER A 56
SHEET
            D 9 GLY A 235 ILE A 238
        3
                                     1 O GLY A 237
                                                      N ILE A 80
SHEET
         4
           D 9 VAL A 257
                          ILE A 260 1 O CYS A 259
                                                      N ILE A 238
         5 D 9 VAL A 287 ILE A 292 1
SHEET
                                       O GLY A 288
                                                      N LEU A 258
SHEET
          D 9 PHE A 308 ILE A 311 1
         6
                                       O LYS A 310
                                                      N ALA A 289
SHEET
        7
           D 9 VAL A 355 ASP A 358 1
                                        0
                                           CYS A 356
                                                      N ILE A 311
           D 9 PHE A 377 LEU A 380 1 O PHE A 377
SHEET
        8
                                                      N SER A 357
           D 9 LEU A 54 SER A 56 1 N VAL A 55
SHEET
        9
                                                      O ILE A 378
SHEET
          E 3 LYS A 394 ILE A 397 0
        1
SHEET
        2 E 3 SER A 400 TRP A 406 -1 O MET A 402
                                                      N VAL A 395
SHEET
        3 E 3 ASP A 434 PRO A 438 -1 O SER A 435
                                                     N TYR A 405
SSBOND
       1 CYS A 26 CYS A 459
CISPEP
       1 GLY A 290 ASN A 291
                                           0
                                                    0.82
CRYST1 155.070 155.070 155.070 90.00 90.00 90.00 P 4 3 2
ORIGX1
           1.000000 0.000000 0.000000 0.00000
ORIGX2
           0.000000 1.000000 0.000000
                                            0.00000
           0.000000 0.000000 1.000000
ORIGX3
                                            0.00000
          0.006449 0.000000 0.000000
SCALE1
                                            0.00000
SCALE2
           0.000000 0.006449 0.000000
                                            0.00000
SCALE3
           0.000000 0.000000 0.006449
                                             0.00000
         1 N ALA A 2
                              55.246 75.030 36.667 1.00 28.12
56.014 73.998 35.916 1.00 26.83
MOTA
                                                                         N
         2 CA ALA A
MOTA
                       2
                                                                         С
         3 C ALA A
ATOM
                       2
                              57.303 73.637 36.651 1.00 27.59
                                                                         С
         4 0
MOTA
                      2
                              57.744 74.364 37.542 1.00 26.06
               ALA A
ATOM
         5 CB ALA A
                      2
                              56.331 74.512
                                             34.522 1.00 27.30
                                                                         C
MOTA
         6 N LYS A
                                             36.272 1.00 27.55
                      3
                              57.901
                                     72.510
                                                                         N
ATOM
         7 CA LYS A
                      3
                              59.139
                                     72.052 36.891 1.00 28.66
                                                                         C
ATOM
         8 C
               LYS A
                      3
                            60.304
                                     72.241
                                             35.923 1.00 28.28
                           60.213 71.877 34.751 1.00 28.88
59.022 70.571 37.276 1.00 30.08
60.256 70.001 37.985 1.00 34.20
60.835 68.809 37.222 1.00 37.41
         9 0
MOTA
               LYS A
                      3
                                                                         0
MOTA
        10 CB LYS A
                       3
                                                                         С
MOTA
        11 CG
               LYS A
                       3
                                                                         C
ATOM
        12 CD LYS A
                      3
                              60.835 68.809 37.222 1.00 37.41
```

ATOM	1	.3	CE	LYS	A	3		61.981	68.154	37.977	1.00	38.58		С
ATOM	` 1	4	NZ ·	LYS	Α	3		63.081	69.118	38.256	1.00	40.73		N
MOTA	. 1	.5	N	TYR	Α	4		61.396	72.809	36.424	1.00	27.63		N
ATOM	1	.6	CA	TYR	Α	4		62.589	73.060	35.617		27.84		С
ATOM	1	.7	С	TYR	A	4		63.789	72.257	36.120	1.00	29.05		C
ATOM	1	.8	0	TYR	Α	4		63.729	71.620	37.168		28.98		0
ATOM			СВ	TYR		4		62.906	74.559	35.635		26.14		C
ATOM			CG	TYR		4		61.816	75.386	34.994	1.00			C
ATOM			CD1	TYR		4		61.746	75.528	33.607	1.00			C
ATOM			CD2	TYR		4		60.819	75.981	35.769	1.00			C
ATOM			CE1	TYR		4		60.707	76.243	33.007		24.96		C
ATOM			CE2	TYR		4		59.773	76.699	35.177		26.60		C
ATOM			CZ	TYR		4		59.726	76.824	33.799		25.65		C
ATOM			OH	TYR		4		58.698	77.523	33.215	1.00			0
ATOM			N	TYR		5		64.880	72.288	35.362	1.00			N
ATOM			CA	TYR		5		66.082	71.556	35.732		31.29		C
MOTA			C	TYR		5		67.275	72.487	35.860		32.27		C
MOTA			0	TYR		5		67.313	73.551	35.241	1.00			
ATOM			CB	TYR		5		66.370						0
ATOM	3		CG	TYR		5			70.467	34.700		30.15		C
ATOM								65.246	69.467	34.568		30.45		C
						5		64.076	69.789	33.876	1.00			C
ATOM	3			TYR		5		65.338	68.203	35.158	1.00			C
ATOM						5		63.028	68.879	33.775	1.00		•	C
ATOM			CE2			5		64.298	67.289	35.064	1.00			C
ATOM			CZ	TYR		5		63.147	67.632	34.372	1.00			C
ATOM			OH	TYR		5	•	62.122	66.728	34.277		29.57		0
ATOM	3		N	ASN		6		68.249	72.079	36.667	1.00			N
ATOM	4		CA	ASN		6		69.445	72.880	36.903	1.00			С
ATOM	4		C	ASN		6		70.421	72.883	35.732	1.00			С
ATOM	4		0	ASN		6		71.190	73.827	35.569	1.00			0
ATOM	4		CB	ASN		6		70.158	72.380	38.162	1.00			С
ATOM			CG .	ASN		6		69.322	72.563	39.417		40.37		C
ATOM	4			ASN		6		69.335	71.716	40.315	1.00			0
ATOM	4			ASN		6		68.597	73.679	39.493	1.00			N
MOTA			N	GLU		7		70.388	71.839	34.912	1.00			N
MOTA	4		CA	GLU		7		71.301	71.749	33.774	1.00	30.55		С
ATOM	4		С	GLU		7		70.588	71.404	32.477	1.00			C
MOTA	5		0	GLU		7		69.563	70.724	32.483	1.00			0
MOTA	5		CB	GLU		7		72.365	70.671	34.030	1.00			C
MOTA	]5			GLU		7		73.323	70.926	35.203	1.00	36.46		C
ATOM	5		CD	GLU		7		74.235	72:121	34.978	1.00	38.59		С
ATOM				GLU		. 7		74.649	72.348	33.821	1.00	39.18		0
MOTA	5		OE2	GLU		7		74.552	72.828	35.961	1.00	41.76		0
MOTA			N	PRO		8		71.125	71.868	31.339	1.00	26.18		N
ATOM			CA	PRO		8		70.484	71.549	30.062	1.00			C
ATOM	5	8	C	PRO		8		70.830	70.098	29.736	1.00	25.66		С
MOTA	5	9	0	PRO		8		71.796	69.561	30.281	1.00	25.70		0
MOTA	6	0	CB	PRO	А	8		71.140	72.530	29.094	1.00	25.89		C
ATOM	6	1	CG	PRO	Α	8		72.531	72.678	29.661	1.00	24.82		С
MOTA	6	2	CD	PRO	A	8		72.270	72.780	31.149	1.00	25.95		C
ATOM	6	3	N	CYS	Α	9		70.053	69.457	28.869	1.00	25.32		N
MOTA	6	4	CA	CYS	A	9		70.342	68.074	28.501	1.00	25.12		C
ATOM	6	5	C	CYS	Α	9		71.405	68.030	27.396	1.00	24.58		C
ATOM	6	6	0	CYS	A	9		71.599	69.009	26.674	1.00	24.57		0
MOTA	6	7	CB	CYS	Α	9		69.058	67.354	28.064	1.00	25.98		C
MOTA	6	8	SG	CYS	Α	9		68.140	68.110	26.701	1.00			s
ATOM	6	9	N	HIS	A	10		72.087	66.895	27.267	1.00			N

ATOM	70	CA	HIS		10	73.159	66.735	26.284	1.00 22.97	•	С
ATOM	71	C	HIS		10	73.016	65.458	25.450	1.00 23.29		C
ATOM	72	0	HIS		10	72.389	64.491	25.886	1.00 22.16		0
ATOM	. 73	CB	HIS		10	74.505	66.695	27.013	1.00 23.38		C
ATOM	74	CG	HIS		10	74.767	67.892	27.874	1.00 24.01		C
ATOM	75		HIS		10	75.212	69.094	27.364	1.00 23.71		N
MOTA	76		HIS		10	74.645	68.071	29.211	1.00 23.36		С
ATOM	77		HIS	A	10	75.353	69.962	28.351	1.00 22.56		C
MOTA	78	NE2	HIS	A	10	75.015	69.366	29.481	1.00 23.59		N
MOTA	79	N	THR	A	11	73.605	65.462	24.255	1.00 23.11		N
MOTA	80	CA	THR		11	73.573	64.300	23.362	1.00 23.58		C
MOTA	81	C	THR		11	74.920	63.571	23.464	1.00 23.26		С
MOTA	82	0	THR		11	75.858	64.093	24.061	1.00 22.66		0
MOTA	83	CB	THR	Α	11	73.360	64.719	21.889	1.00 24.09	•	С
ATOM	84	OG1			11	74.439	65.562	21.475	1.00 25.91		0
ATOM	85	CG2			11	72.049	65.480	21.727	1.00 25.24		С
ATOM	86	N	PHE		12	75.017	62.377	22.881	1.00 23.30		N
ATOM	87	CA	PHE	Α	12	76.262	61.609	22.931	1.00 24.87		С
ATOM	88	C	PHE	Α	12	77.458	62.328	22.304	1.00 26.16		С
ATOM	89	0	PHE		12	78.596	62.112	22.713	1.00 26.04		0
MOTA	90	CB	PHE	Α`	12	76.096	60.243	22.249	1.00 23.25		C
ATOM	91	CG	PHE		12	75.216	59.284	23.004	1.00 23.37		С
MOTA	92	CD1	PHE	Α	12	75.362	59.119	24.377	1.00 22.09		C
MOTA	93	CD2			12	74.253	58.537	22.337	1.00 22.79		С
ATOM	94	CE1	PHE	А	12	74.560	58.223	25.078	1.00 23.40		C
MOTA	95	CE2	PHE		12	73.443	57.634	23.027	1.00 24.01		С
MOTA	96	CZ	PHE		12	73.596	57.476	24.399	1.00 22.98		C
ATOM	97	N	ASN		13	77.202	63.173	21.310	1.00 26.96		N
MOTA	98	CA	ASN		13	78.2 <b>7</b> 3	63.905	20.637	1.00 28.09		C
ATOM	99	С	ASN		13	78.998	64.901	21.533	1.00 26.75		C
ATOM	100	0	ASN		13	80.044	65.420	21.152	1.00 27.23		0
ATOM	101	CB	ASN		13	77.734	64.663	19.417	1.00 31.04		C
MOTA	102	CG	ASN		13	77.622	63.787	18.183	1.00 36.11		С
ATOM	103		ASN		13	78.522	63.000	17.883	1.00 39.98		0
ATOM	104	ND2	ASN		13	76.526	63.934	17.448	1.00 38.57		N
ATOM	105	N	GLU		14	78.445	65.178	22.710	1.00 25.07		N
ATOM	106	CA	GLU		14	79.060	66.136	23.621	1.00 25.01		С
ATOM	107	С	GLU		14	79.976	65.483	24.650	1.00 25.17		С
ATOM	108	0	GLU		14	80.464	66.148	25.563	1.00 26.57		0
ATOM	109	CB	GLU		14	77.976	66.937	24.348	1.00 25.02		С
MOTA	110	CG	GLU		14	. 77.000	67.638	23.420	1.00 25.34		C
ATOM	111	CD	GLU		14	75.926	68.401	24.169	1.00 25.36		C
MOTA	112		GLU		14	76.272	69.314	24.947	1.00 25.19		0
MOTA	113		GLU		14	74.734	68.083	23.978	1.00 26.80		0
ATOM	114	N	TYR		15	80.229	64.189	24.499	1.00 24.38		N
ATOM	115	CA	TYR		15	81.067	63.487	25.455	1.00 23.13		C
ATOM	116	C,	TYR		15	82.248	62.754	24.856	1.00 23.75		C
ATOM ·	117	0	TYR		15	82.230	62.360	23.691	1.00 24.15		0
MOTA	118	CB	TYR		15	80.224	62.478	26.238	1.00 22.70		C
ATOM	119	CG	TYR		15	79.201	63.097	27.153	1.00 23.45		C
ATOM	120		TYR		15	79.519	63.416	28.474	1.00 23.71		C
ATOM	121		TYR		15	77.909	63.361	26.702	1.00 24.00		C
ATOM	122		TYR		15	78.571	63.977	29.326	1.00 25.23		C
ATOM	123		TYR		15	76.954	63.927	27.544	1.00 25.30		C
ATOM	124	CZ	TYR		15	77.288	64.231	28.851	1.00 25.69		С
ATOM	125	OH	TYR		15	76.342	64.793	29.680	1.00 29.22		0
MOTA	126	N	LEU	A	16	83.273	62.570	25.681	1.00 24.09		N

ATOM	127	CA	LEU	Α	16	84.470	61.830	25.301	1.00 24.11	L	С
MOTA	128	C	LEU	A	16	84.866	61.010	26.519	1.00 23.10	)	C
MOTA	129	0	LEU	Α	16	84.525	61.360	27.649	1.00 22.07		0
MOTA	130	CB	LEU		16	85.625	62.767	24.922	1.00 24.98	}	С
MOTA	131	CG	LEU		16	85.590	63.480	23.569	1.00 26.50	)	С
ATOM	132		LEU		16	86.770	64.421	23.467	1.00 28.14	<u> </u>	C
ATOM	133		LEU		16	85.635	62.471	22.444	1.00 28.66	; ;	С
ATOM	134	N	LEU		17	85.572	59.913	26.279	1.00 23.04	:	N
ATOM	135	CA	LEU		17	86.047	59.040	27.346	1.00 23.77		C
ATOM	136	C	LEU		17	87.512	59.362	27.630	1.00 23.70		C
ATOM	137	0	LEU		17	88.301	59.540	26.706	1.00 23.54		0
ATOM	138	CB	LEU		17	85.929	57.569	26.923	1.00 22.71		C
ATOM	139	CG	LEU		17	84.511	56.990	26.882	1.00 23.40		C
ATOM ATOM	140 141		LEU		17	84.480	55.739	26.022	1.00 23.07		С
ATOM	141	CD2	_		17	84.047	56.698	28.301	1.00 21.29		C
ATOM	143	N CA	ILE		18	87.860	59.456	28.909	1.00 24.51		N
ATOM	143	CA	ILE		18	89.236	59.720	29.313	1.00 24.55		С
ATOM	145	0	ILE		18 18	89.803	58.357	29.705	1.00 24.94		С
ATOM	145	CB	ILE		18	89.236	57.670	30.545	1.00 25.77		0
ATOM	147	CG1			18	89.279 88.798	60.687	30.509	1.00 24.40		C
ATOM	148	CG2			18	90.696	62.071 60.750	30.054	1.00 25.23		C
ATOM	149	CD1			18	88.754	63.115	31.089 31.149	1.00 24.00		C
ATOM	150	N	PRO		19	90.921	57.942	29.089	1.00 26.14		C
ATOM	151	CA	PRO		19	91.519		29.402	1.00 24.65 1.00 26.08		N
ATOM	152	C	PRO		19	91.842	56.372	30.868	1.00 26.08		C
ATOM	153	Ō	PRO		19	92.120	57.288	31.646	1.00 25.01		C
ATOM	154	CB	PRO		19	92.787	56.610	28.533	1.00 25.83		0
ATOM	155	CG	PRO		19	92.431	57.503	27.375	1.00 26.14		C C
ATOM	156	CD	PRO		19	91.708	58.646	28.061	1.00 24.66		C
ATOM	157	N	GLY		20	91.792	55.092	31.221	1.00 25.78		N
MOTA	158	CA	GLY		20	92.118	54.654	32.564	1.00 25.89		C
ATOM	159	C	GLY	Α	20	93.331	53.748	32.425	1.00 26.31		C
ATOM	160	0	GLY	Α	20	93.940	53.671	31.353	1.00 26.09		Ö
ATOM	161	N	LEU	Α	21	93.692	53.052	33.492	1.00 27.91		N
ATOM	162	CA	LEU	Α	21	94.842	52.161	33.436	1.00 28.51		C ·
MOTA	163	С	LEU	A	21	94.522	50.917	32.626	1.00 28.22		C
ATOM	164	0	LEU		21	93.599	50.178	32.950	1.00 28.84		O
MOTA	165	CB	LEU		21	95.281	51.748	34.850	1.00 28.54		C
ATOM	166	CG	LEU		21	96.424	50.721	34.929	1.00 28.79		С
MOTA	167		LEU		21	97.661	51.272	34.230	1.00 25.50		С
ATOM	168		LEU		21	96.726	50.390	36.394	1.00 28.73		C
ATOM	169	N	SER		22	95.284	50.697	31.562	1.00 29.18		N
ATOM	170	CA	SER		22	95.099	49.525	30.725	1.00 30.50		C
MOTA	171	C	SER		22	96.101	48.467	31.171	1.00 32.47		С
ATOM	172	0	SER		22	97.310	48.684	31.107	1.00 31.83		0
ATOM ATOM	173	CB	SER		22	95.340	49.874	29.259	1.00 30.15		C
ATOM	174	OG N	SER		22	94.432	50.858	28.813	1.00 31.65		0
ATOM	175 176	N CA	THR		23	95.595	47.327	31.630	1.00 35.11		N
ATOM	177	CA	THR THR		23	96.451	46.237	32.090	1.00 36.70		C
ATOM	178	0.	THR		23	96.864	45.327	30.941	1.00 37.53		C
ATOM	179	CB	THR		23 23	96.241	45.331	29.879	1.00 38.20		0
ATOM	180		THR		23	95.741	45.392	33.155	1.00 37.23		C
ATOM	181		THR .		23	94.462 95.552	44.985	32.660	1.00 40.43		0
ATOM	182	N	VAL .		24	97.919	46.191 44.547	34.429	1.00 37.20		C
ATOM	183	CA	VAL .		24	98.425		31.159	1.00 38.34		N
	-00	O.13	V434 .	• •	~ =	20.443	43.636	30.135	1.00 38.85		C

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MOTA	184	C	VAL	A	24	97.396	42.605	29.666	1.00 39.73		С
ATOM	185	0	VAL	Α	24	97.401	42.203	28.499	1.00 39.77		0
ATOM	186	CB	VAL	Α	24	99.700	42.886	30.625	1.00 39.23		C
ATOM	187	CG1	VAL	Α	24	100.851	43.871	30.800	1.00 38.15		C
ATOM	188	CG2	VAL	Α	24	99.418	42.167	31.938	1.00 38.35		C
MOTA	189	N	ASP	Α	25	96.506	42.186	30.560	1.00 40.55		N
MOTA	190	CA	ASP	A	25	95.503	41.195	30.186	1.00 43.23		C
MOTA	191	С	ASP	Α	25	94.328	41.733	29.370	1.00 42.88		C
MOTA	192	0	ASP	Α	25	93.485	40.951	28.933	1.00 43.24		0
MOTA	193	CB	ASP	Α	25	94.956	40.476	31.425	1.00 45.78		C
MOTA	194	CG	ASP	A	25	94.301	41.421	32.405	1.00 48.75		C
ATOM	195	OD1	ASP	Α	25	93.333	41.010	33.083	1.00 49.75		0
MOTA	196	OD2	ASP	Α	25	94.764	42.574	32.503	1.00 50.54		0
ATOM	197	N	CYS	Α	26	94.257	43.045	29.150	1.00 42.32		N
ATOM	198	CA	CYS	Α	26	93.137	43.581	28.377	1.00 41.35		C
ATOM	199	C	CYS	Α	26	93.440	43.763	26.903	1.00 41.34		C
ATOM	200	0	CYS	Α	26	94.067	44.738	26.496	1.00 41.54		0
MOTA	201	CB	CYS	Α	26	92.640	44.924	28.943	1.00 39.84		C
ATOM	202	SG	CYS	Α	26		. 45.372	28.462	1.00 36.85		s
MOTA	203	N	ILE	Α	27	92.992	42.802	26.108	1.00 42.52		N
ATOM	204	CA	ILE	Α	27	93.142	42.857	24.664	1.00 43.62		C
ATOM	205	С	ILE	Α	27	91.725	42.630	24.152	1.00 44.10		C
ATOM	206	0	ILE	Α	27	90.935	41.930	24.789	1.00 43.64		0
MOTA	207	CB	ILE	Α	27	94.086	41.748	24.125	1.00 45.23		C
ATOM	208	CG1	ILE	Α	27	93.613	40.374	24.601	1.00 45.47		C
MOTA	209	CG2	ILE	A	27	95.519	42.019	24.579	1.00 44.91		C
ATOM	210	CD1	ILE	Α	27	94.479	39.224	24.114	1.00 47.61		C
ATOM	211	N	PRO	Α	28	91.377	43.235	23.010	1.00 44.56		N
ATOM	212	CA	PRO	Α	28	90.041	43.090	22.429	1.00 44.54		C
ATOM	213	С	PRO	Α	28	89.474	41.673	22.450	1.00 44.69		C
ATOM	214	0	PRO	Α	28	88.312	41.471	22.801	1.00 44.73		0
ATOM	215	CB	PRO	Α	28	90.233	43.625	21.016	1.00.45.21		C
ATOM.	216	CG	PRO	Α	28	91.205	44.738	21.239	1.00 44.60		C
ATOM	217	CD	PRO	Α	28	92.221	44.104	22.170	1.00 44.85		C
MOTA	218	N	SER	A	29	90.292	40.692	22.082	1.00 44.42		И
ATOM	219	CA	SER	Α	29	89.835	39.307	22.048	1.00 43.86		C
MOTA	220	C	SER	Α	29	89.390	38.767	23.405	1.00 42.44		C
MOTA	221	0	SER	A ·	29	88.605	37.821	23.468	1.00 43.23		0
MOTA	222	CB	SER	Α	29	90.926	38.400	21.455	1.00 45.84		C
MOTA	223	OG	SER	Α	29	92.107	38.401	22.241	1.00 48.98		0
MOTA	224	N	ASN	Α	30	89.878	39.357	24.491	1.00 40.37		N
MOTA	225	CA	ASN	Α	30	89.489	38.892	25.819	1.00 39.43		C
MOTA	226	C	ASN	A	30	88.330	39.695	26.417	1.00 37.05		C
ATOM	227	0	ASN	Α	30	87.912	39.442	27.548	1.00 36.90		0
ATOM .	228	CB	ASN	Α	30	90.677	38.942	26.788	1.00 41.28		C
MOTA	229	CG	ASN	A	30	91.830	38.061	26.348	1.00 44.29		C
MOTA	230	OD1	ASN	A	30	91.638	37.064	25.648	1.00 45.64		0
ATOM	231	ND2	ASN	Α	30	93.040	38.417	26.773	1.00 44.79		N
ATOM	232	N	VAL .	Α	31	87.817	40.666	25.668	1.00 34.05		N
MOTA	233	CA	VAL .	A	31	86.716	41.478	26.169	1.00 31.36		C
ATOM	234	C	VAL .	A	31	85.404	40.711	26.051	1.00 30.32		C
ATOM	235	0	VAL .	A	31	85.090	40.149	25.005	1.00 28.53		0
ATOM	236	CB	VAL .	A	31	86.615	42.823	25.404	1.00 31.14		C
MOTA	237	CG1	VAL .	A	31	85.429	43.641	25.919	1.00 29.88		C
MOTA	238	CG2	VAL .	A	31	87.910	43.612	25.579	1.00 29.52		C
MOTA	239	N	ASN .		32	84.653	40.680	27.144	1.00 29.79		N
MOTA	240	CA	ASN .	A	32	83.369	39.987	27.195	1.00 30.76		C
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MOTA	241	C	ASN		32	82.246	41.013	27.030	1.00 30.01		С
MOTA	242	0	ASN		32	82.095	41.908	27.860	1.00 29.60		0
ATOM	243	CB	ASN	·A	32	83.244	39.266	28.541	1.00 32.62		С
ATOM	244	CG	ASN	A	32	81.916	38.549	28.716	1.00 34.80		С
MOTA	245	OD1	ASN	Α	32	81.640	38.004	29.786	1.00 38.96		0
MOTA	246	ND2	ASN	Α	32	81.093	38.538	27.676	1.00 32.90		N
MOTA	247	N	LEU	Α	33	81.458	40.872	25.964	1.00 29.61		N
MOTA	248	CA	LEU	Α	33	80.361	41.798	25.677	1.00 29.44		С
MOTA	249	C	LEU	Α	33	78.961	41.292	26.050	1.00 29.73		С
MOTA	250	0	LEU	Α	33	77.955	41.805	25.555	1.00 29.64		0
MOTA	251	CB	LEU	A	33	80.397	42.176	24.191	1.00 30.47		C
MOTA	252	CG	LEU	A	33	80.910	43.558	23.761	1.00 31.37		С
ATOM	253	CD1	LEU	Α	33	81.975	44.091	24.699	1.00 30.40		С
ATOM	254	CD2	LEU	Α	33	81.439	43.446	22.350	1.00 31.39		C
MOTA	255	N	SER	Α	34	78.892	40.289	26.920	1.00 28.68		N
ATOM	256	CA	SER	Α	34	77.605	39.752	27.360	1.00 28.45		C
MOTA	257	С	SER	А	34	76.885	40.800	28.197	1.00 26.82		C
ATOM	258	0	SER	Α	34	77.521	41.633	28.840	1.00 27.22		ō
MOTA	259	CB	SER	A	34	77.812	38.502	28.216	1.00 28.51		Ċ
MOTA	260	OG	SER	A	34	78.504	37.518	27.477	1.00 35.24		Ö
MOTA	261	N	THR	Α	35	75.561	40.750	28.209	1.00 24.82		N
MOTA	262	CA	THR	Α	35	74.795	41.709	28.982	1.00 23.94		C
MOTA	263	С	THR	Α	35	73.380	41.170	29.201	1.00 24.11		C
ATOM	264	0	THR	Α	35	72.834	40.470	28.349	1.00 25.00		Ö
ATOM	265	CB	THR	Α	35	74.752	43.084	28.251	1.00 24.28		C
MOTA	266	OG1	THR	Α	35	74.409	44.117	29.181	1.00 24.41		0
MOTA	267	CG2	THR	A	35	73.728	43.069	27.126	1.00 21.95		C
ATOM	268	N	PRO	Α	36	72.776	41.478	30.358	1.00 23.32		N
ATOM .	269	CA	PRO	Α	36	71.419	41.023	30.687	1.00 22.99		C
ATOM	270	C	PRO	Α	36	70.304	41.697	29.881	1.00 24.25		C
ATOM	271	0	PRO	A	36	70.321	42.912	29.670	1.00 23.91		0
MOTA	272	CB	PRO	A	36	71.309	41.328	32.177	1.00 22.91		C
MOTA	273	CG	PRO	A	36	72.159	42.567	32.321	1.00 22.08	•	C
ATOM	274	CD	PRO	Α	36	73.370	42.236	31.475	1.00 22.10		C
ATOM	275	N	LEU	Α	37	69.329	40.900	29.447	1.00 24.03		N
MOTA	276	CA	LEU	A	37	68.201	41.407	28.677	1.00 24.03		C
ATOM	277	C ·	LEU	Α	37	66.974	41.670	29.552	1.00 24.86		C
ATOM	278	0	LEU	Α	37	66.293	42.684	29.385	1.00 25.14		Ö
ATOM	279	ÇВ	LEU	Α	37	67.825	40.420	27.567	1.00 24.13		C.
ATOM	280	CG	LEU	Α	37		40.862	26.614	1.00 25.46	•	C.
ATOM	281	CD1	LEU	Α	37	67.191	42.043	25.759	1.00 24.90		C
ATOM	282	CD2	LEU	Α	37	66.306	39.698	25.708	1.00 25.09		C
MOTA	283	N	VAL		38	66.691	40.767	30.487	1.00 24.24		N
ATOM	284	CA	VAL		38	65.525	40.920	31.347	1.00 24.00		C
ATOM	285	С	VAL		38	65.889	40.950	32.820	1.00 25.63		C
ATOM	286	0	VAL	Α	38	66.942	40.454	33.215	1.00 26.92		0
ATOM	287	CB	VAL	Α	38	64.488	39.802	31.074	1.00 24.41		C
MOTA	288	CG1	VAL	Α	38	64.014	39.890	29.623	1.00 21.19		C
MOTA	289	CG2	VAL	Α	38	65.100	38.427	31.349	1.00 23.21		C
MOTA	290	N	LYS		39	65.003	41.527	33.629	1.00 25.88		N
MOTA	291	CA	LYS		39	65.240	41.686	35.060	1.00 27.51		C
MOTA	292	С	LYS		39	65.422	40.413	35.869	1.00 28.51		C
ATOM	293	0	LYS		39	64.916	39.351	35.513	1.00 29.00		0
MOTA	294	CB	LYS		39	64.121	42.513	35.697	1.00 27.27		C
MOTA	295	CG	LYS		39	62.754	41.843	35.661	1.00 27.27		C
ATOM	296	CD	LYS		39	61.751	42.595	36.514	1.00 27.78		C
MOTA	297	CE	LYS		39	60.369	41.943	36.448	1.00 29.12		C
							-				C

MOTA	298	NZ	LYS	A	39	59.401	42.617	37.361	1.00	28.02	N
ATOM	299	N	PHE	A	40	66.152	40.556	36.973	1.00	28.42	N
ATOM	300	CA	PHE	A	40	66.439	39.470	37.893	1.00	29.14	C
MOTA	301	C	PHE	A	40	66.668	40.063	39.278	1.00	30.30	С
ATOM	302	0	PHE		40	66.794	41.278	39.421		30.54	0
MOTA	303	СВ	PHE		40	67.687	38.697	37.449		28.10	C
ATOM	304	CG	PHE		40	68.913	39.558	37.251	1.00	27.25	C
ATOM	305		PHE		40	69.163	40.167	36.023		25.59	C
ATOM	306		PHE		40	69.824	39.743	38.287		25.17	C
ATOM	307		PHE		40	70.304	40.944	35.830		25.72	C
ATOM	308		PHE		40	70.968	40.518	38.106		25.52	C
ATOM	309	CZ	PHE					36.873		26.27	
MOTA		N			40	71.211	41.120				C
	310		GLN		41 .	66.713	39.200	40.291		31.34	N
ATOM	311	CA	GLN		41	66.927	39.622	41.672		33.56	C
ATOM	312	C	GLN		41	68.408	39.585	41.998		32.76	C
ATOM	313	0	GLN		41	69.183	38.929	41.305		32.65	0
ATOM	314	CB	GLN		41	66.190	38.685	42.641		36.73	C
MOTA	315	CG	GLN	А	41	64.681	38.719	42.523		42.60	C
MOTA	316	CD	GLN		41	64.087	40.002	43.073	1.00	45.09	C
MOTA	317	OE1	GLN	Α	41	62.956	40.359	42.749	1.00	48.80	0
MOTA	318	NE2	GLN	А	41	64.842	40.693	43.921	1.00	48.01	· <b>N</b>
ATOM	319	N	LYS	Α	42	68.798	40.280	43.061	1.00	32.91	N
ATOM	320	CA	LYS	Α	42	70.191	40.291	43.471	1.00	34.34	C
ATOM	321	Ċ	LYS	A	42	70.670	38.865	43.747	1.00	34.29	C
MOTA	322	0	LYS		42	69.934	38.055	44.311		32.99	0
MOTA	323	CB	LYS		42	70.382	41.129	44.731		35.20	C
MOTA	324	CG	LYS		42	71.849	41.328	45.053		39.21	C
ATOM	325	CD	LYS		42	72.079	42.234	46.244		42.37	C
ATOM	326	CE	LYS		42	71.760	41.547	47.549		42.56	C
ATOM	327	NZ	LYS		42	72.329	42.327	48.680		43.58	N
ATOM	328	N	GLY		43	71.902					
							38.568	43.345		34.17	N
MOTA	329	CA	GLY		43	72.457	37.244	43.565		34.57	C
ATOM	330	C	GLY		43	72.186	36.277	42.431		34.77	C
ATOM	331	0	GLY		43	72.784	35.202	42.361		34.67	0
ATOM	332	N	GLN		44	71.282	36.655	41.538		35.36	N
MOTA	333	CA	GLN		44	70.942	35.810	40.403		36.05	C
MOTA	334	C	GLN		44	71.551	36.364	39.123		35.80	C
ATOM	335	0	GLN		44	72.230	37.390	39.138		35.18	0
MOTA	336	CB	GLN	Α	44	69.422	35.740	40.228	1.00	38.46	C
ATOM	337	CG-	GĽŅ	A	44	68.644	35.556	41.517	1.00	42.54	C
ATOM	338	CD	GLN	Α	44	67.145	35.481	41.281	1.00	44.54	C
MOTA	339	OE1	GLN	Α	44	66.583	36.271	40.517	1.00	46.34	0
ATOM	340	NE2	GLN	A	44	66.487	34.539	41.945	1.00	44.29	N
ATOM	341	N	GLN	Α	45	71.299	35.664	38.022	1.00	35.96	N
ATOM	342	CA	GLN	Α	45	71.759	36.055	36.695	1.00	36.42	C
MOTA	343	C	GLN	Α	45	70.469	36.221	35.907		35.19	С
MOTA	344	0	GLN		45	69.435	35.682	36.293		35.44	0
MOTA	345	CB	GLN		45	72.586	34.943	36.039		39.65	C
ATOM	346	CG	GLN		45	73.865	34.569	36.763		44.40	c
ATOM	347	CD	GLN		45	74.951	35.614	36.610		47.78	C
ATOM	348		GLN		45	75.471	35.834	35.510		50.39	o
ATOM	349	NE2			45	75.303	36.266	37.714		48.43	И
MOTA	350	N	SER		46	70.519	36.266	34.812		32.83	
ATOM	351	CA	SER		46						N
ATOM		CA				69.333	37.154	33.995		32.14	C
	352		SER		46	69.040	35.856	33.244		32.13	C
ATOM	353	0	SER		46	69.962	35.137	32.864		32.53	0
MOTA	354	CB	SER	A	46	69.554	38.289	32.996	1.00	29.54	С

ATOM	355	OG	SER	А	46	68.415	38.451	32.179	1.00 28.	47		0
MOTA	356	N	GLU	A	47	67.762	35.562	33.032	1.00 32.	14		N
ATOM	357	CA	GLU	A	47	67.364	34.355	32.318	1.00 32.	15		С
MOTA	358	C	GLU		47	67.768	34.441	30.856	1.00 31.			С
ATOM	359	0	GLU		47	67.865	33.424	30.169	1.00 30.	42		0
ATOM	360	CB	GLU		47	65.853	34.154	32.418	1.00 34.			С
ATOM	361	CG	GLU		47	65.358	33.856	33.823	1.00 37.			C
ATOM	362	CD	GLU		47	63.844	33.834	33.905	1.00 41.			С
ATOM	363	OE1			47	63.226	32.981	33.231	1.00 43.			0
MOTA	364	OE2	GLU		47	63.271	34.671	34.639	1.00 43.			0
ATOM	365	N	ILE		48	67.978	35.663	30.373	1.00 30.			N
ATOM	366	CA	ILE		48	68.392	35.871	28.990	1.00 29.			C
ATOM	367	C	ILE		48	69.551	36.863	28.923	1.00 28.			C
ATOM	368	0	ILE		48	69.434	38.010	29.354	1.00 27.			0
ATOM	369	CB	ILE		48	67.241	36.415	28.113	1.00 29.			C
ATOM	370	CG1	ILE		48	66.068	35.430	28.102	1.00 29.			C
ATOM ATOM	3.71	CG2	ILE		48	67.744	36.639	26.687	1.00 28.			C
	372				48	64.865	35.915	27.302	1.00 29.3			C
ATOM ATOM	373 374	N CA	ASN ASN		49	70.676	36.412	28.388	1.00 27.			N
ATOM	375	CA C	ASN		49 49	71.839 72.251	37.271	28.258	1.00 28.		,	C
ATOM	376	0	ASN		49	72.436	37.351 36.328	26.798 26.143	1.00 28.			C
ATOM	377	CB	ASN		49	72.436	36.326	29.101	1.00 30.			0 C
ATOM	378	CG	ASN		49	72.738	36.847	30.592	1.00 27.			C
ATOM	379		ASN		49	72.730	37.914	31.176	1.00 26.			0
ATOM	380		ASN		49	72.317	35.752	31.211	1.00 27.			N
ATOM	381	N	LEU		50	72.317	38.569	26.281	1.00 27.			N
ATOM	382	CA	LEU		50	72.795	38.760	24.899	1.00 27.			C
ATOM	383	C	LEU		50	74.302	38.496	24.876	1.00 26.			C
ATOM	384	0	LEU		50	74.964	38.644	25.900	1.00 25.			0
ATOM	385	CB	LEU		50	72.530	40.203	24.454	1.00 26.			C
ATOM	386	CG	LEU		50	71.098	40.734	24.549	1.00 27.			c
ATOM	387	CD1	LEU		50	71.071	42.216	24.160	1.00 25.			C
ATOM	388		LEU		50	70.190	39.917	23.632	1.00 27.			C
ATOM	389	N	LYS		51	74.837	38.100	23.723	1.00 27.			N
ATOM	390	CA	LYS	A	51	76.275	37.859	23.585	1.00 29.			С
ATOM	391	C	LYS		51	76.941	39.189	23.217	1.00 27.	91		С
ATOM	392	0	LYS	Α	51	78.128	39.397	23.472	1.00 28.	86		0
MOTA	393	CB	LYS	A	51	76.564	36.813	22.496	1.00 30.	79		C
ATOM	394	CG	LYS	A	51	76.813	35.389	23.004	1.00 33.	79		C
ATOM	395	CD.	LYS	A	51	75.558	34.739	23.541	1.00 36.	94 :		С
MOTA	396	CE	LYS	Α	51	75.836	33.339	24.093	1.00 39.	15		C
ATOM	397	NZ	LYS	Α	51	76.304	32.377	23.060	1.00 40.	17		N
ATOM	398	N	ILE	Α	52	76.163	40.070	22.590	1.00 26.	85		N
ATOM	399	CA	ILE	Α	52	76.608	41.411	22.216	1.00 24.	81		С
ATOM	400	С	ILE	A	52	75.442	42.326	22.590	1.00 25.	02		С
MOTA	401	0	ILE	A	52	74.276	41.961	22.425	1.00 24.	33		0
ATOM	402	CB	ILE		52	76.950	41.540	20.700	1.00 25.	62		C
MOTA	403		ILE		52	75.738	41.178	19.833	1.00 25.			С
MOTA	404		ILE		52	78.159	40.654	20.370	1.00 25.			С
MOTA	405		ILE		52	75.946	41.460	18.351	1.00 22.			С
ATOM	406	N	PRO		53	75.742	43.527	23.102	1.00 24.			N
ATOM	407	CA	PRO		53	74.732	44.502	23.526	1.00 25.			C
ATOM	408	C	PRO		53	73.979	45.272	22.439	1.00 25.			C
ATOM	409	0	PRO		53	73.644	46.438	22.638	1.00 25.			0
ATOM	410	CB	PRO		53	75.535	45.432	24.426	1.00 23.			C
MOTA	411	CG	PRO	Α	53	76.829	45.526	23.670	1.00 24.	υU		С

ATOM	412	CD	PRO	А	53	77.101	44.079	23.267	1.00 23.34		С
ATOM	413	N	LEU	А	54	73.705	44.633	21.304	1.00 25.11		N
ATOM	414	CA	LEU	Α	54	72.982	45.306	20.229	1.00 24.78		С
ATOM	415	С	LEU	Α	54	71.670	44.607	19.883	1.00 25.72		С
ATOM	416	0	LEU		54	71.613	43.375	19.783	1.00 25.86		0
ATOM	417	СВ	LEU		54	73.842	45.382	18.965	1.00 24.66		C
MOTA	418	CG	LEU		54	75.270	45.925	19.050	1.00 24.20		C
ATOM	419		LEU		54	75.865	45.913	17.660	1.00 22.76		C
ATOM	420		LEU		54	75.288	47.333	19.636	1.00 23.83		C
ATOM	421	N	VAL		55	70.613	45.396	19.721	1.00 24.79		N
			VAL		55		44.866		1.00 24.79		C
ATOM	422	CA				69.315		19.335	1.00 25.45		C
ATOM	423	C .	VAL		55	68.803	45.777	18.220			
ATOM	424	0	VAL		55	69.044	46.988	18.252	1.00 26.82		0
ATOM	425	CB	VAL		55	68.298	44.846	20.519	1.00 24.52		C
MOTA	426		VAL		55	68.889	44.086	21.698	1.00 23.68		C
MOTA	427		VAL		55	67.906	46.263	20.922	1.00 25.10		C
ATOM	428	N	SER		56	68.132	45.197	17.225	1.00 26.09		N
MOTA	429	CA	SER		56	67.603	45.980	16.111	1.00 26.11	•	С
ATOM	430	C	SER		56	66.219	46.532	16.453	1.00 25.25		С
ATOM	431	0	SER	Α	56	65.418	45.877	17.121	1.00 25.67		0
MOTA	432	CB	SER	A	56	67.565	45.135	14.825	1.00 26.43	***	C
MOTA	433	OG	SER	Α.	56	66.749	43.988	14.965	1.00 27.47		0
ATOM	434	N	ALA	A	57	65.957	47.751	15.996	1.00 24.68		N
ATOM	435	CA	ALA	Α	57·	64.710	48.458	16.270	1.00 25.05		C
ATOM	436	C	ALA	Α	57	63.407	47.783	15.820	1.00 25.91		C
ATOM	437	0	ALA	А	57	63.375	47.019	14.853	1.00 25.61		0
MOTA	438	CB	ALA	Α	57	64.797	49.868	15.691	1.00 22.75		C
MOTA	439	N	ILE		58 ·	62.335	48.091	16.544	1.00 25.97		N
MOTA	440	CA	ILE		58	61.002	47.555	16.276	1.00 27.20		C
MOTA	441	C	ILE		58	60.400	48.361	15.124	1.00 27.24		C
ATOM	442	0	ILE		58	59.417	49.088	15.297	1.00 28.19		ō
ATOM	443	CB	ILE		58	60.114	47.696	17.535	1.00 26.40	,	Č
MOTA	444	CG1	ILE		58	60.929	47.293	18.773	1.00 26.10		Ĉ
MOTA	445		ILE		58	58.869	46.829	17.403	1.00 25.39		C
ATOM	446		ILE		58	60.144	47.268	20.061	1.00 25.45		C
ATOM	447	И	MET		59	60.144	48.213	13.945	1.00 23.43		N
ATOM	448	CA	MET		59	60.581	48.965	12.768	1.00 27.85		C
ATOM	449	C .	MET		59	60.419	48.127	11.501	1.00 28.29		C
MOTA	450	0	MET		59	61.177	47.185	11.261	1.00 27.17		0
ATOM	451	CB	MET		59	61.604	50.072	12.503	1.00 27.11		C
MOTA	452	CG	MET		59	61.908	50.946	13.711	1.00 26.18	•	C
MOTA	453	SD	MET		59	63.235	52.128	13.373	1.00 28.54		S
ATOM	454	CE	MET		59	62.471	53.130	12.107	1.00 25.89		C
MOTA	455	N	GLN		60	59.444	48.505	10.679	1.00 29.33		N
MOTA	456	CA	GLN		60	59.163	47.806	9.428	1.00 30.56		C
ATOM	457	C	GLN	А	60	60.372	47.772	8.503	1.00 30.93		С
MOTA	458	0	GLN	Α	60	60.576	46.800	7.783	1.00 31.46		0
MOTA	459	CB	GLN	A	60	58.006	48.479	8.674	1.00 31.20		C
ATOM	460	CG	GLN	Α	60	56.741	48.712	9.491	1.00 32.68		С
MOTA	461	CD	GLN	Α	60	55.654	49.395	8.680	1.00 33.85		C
ATOM	462	OE1			60	55.941	50.208	7.802	1.00 36.50		0
ATOM	463	NE2	GLN		60	54.401	49.079	8.979	1.00 34.24		N
MOTA	464	N	SER		61	61.171	48.834	8.519	1.00 30.66		N
MOTA	465	CA	SER		61	62.332	48.906	7.639	1.00 31.00		C
ATOM	466	C	SER		61	63.619	48.359	8.241	1.00 30.65		Ċ
MOTA	467	0	SER		61	64.695	48.514	7.659	1.00 30.72		0
MOTA	468	CB	SER		61	62.553	50.353	7.185	1.00 30.89		C
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MOTA	469	OG	SER		61	62.658	51.225	8.292	1.00 34.36		0
ATOM	470	N	VAL		62	63.512	47.698	9.388	1.00 30.00		N
MOTA	471	CA	VAL		62	64.696	47.165	10.039	1.00 29.68		C
MOTA	472	С	VAL		62	64.642	45.696	10.449	1.00 30.05		С
MOTA	473	0	VAL		62	65.413	44.880	9.948	1.00 30.69		0
MOTA	474	CB	VAL	А	62	65.046	47.997	11.306	1.00 29.93		C
MOTA	475	CG1	VAL	A	62	66.287	47.418	11.989	1.00 30.22		C
MOTA	476	CG2	VAL	Α	62	65.280	49.460	10.926	1.00 29.24		C
ATOM	477	N	SER	Α	63	63.729	45.364	11.354	1.00 30.78		N
MOTA	478	CA	SER	Α	63	63.641	44.011	11.889	1.00 31.26		С
MOTA	479	C	SER	Α	63	62.664	43.019	11.267	1.00 32.02		C
ATOM	480	0	SER	Α	63	61.535	42.842	11.741	1.00 30.32		0
ATOM	481	CB	SER	Α	63	63.389	44.091	13.400	1.00 30.76		С
ATOM	482	OG	SER	A	63 .	64.420	44.825	14.051	1.00 29.40		0
ATOM	483	N	GLY	Α	64	63.122	42.361	10.211	1.00 32.88		N
ATOM	484	CA	GLY	Α	64	62.320	41.352	9.553	1.00 33.87		С
ATOM	485	С	GLY	Α	64	62.916	40.005	9.925	1.00 35.96		C
ATOM	486	0	GLY	Α	64	63.761	39.932	10.823	1.00 33.92		0
ATOM	487	N	GLU	Α	65	62.501	38.949	9.226	1.00 37.32		N
ATOM	488	ÇA	GLU	Α	65	62.980	37.596	9.493	1.00 39.14		С
ATOM	489	С	GLU	Α	65	64.487	37.461	9.320	1.00 37.65		C
ATOM	490	0	GLU	Α	65	65.175	36.945	10.198	1.00 36.98		0
ATOM	491	CB	GLU	Α	65	62.298	36.591	8.559	1.00 42.54		C
ATOM	492	CG	GLU		65	60.841	36.885	8.260	1.00 48.99		С
ATOM	493	CD	GLU		65	60.245	35.884	7.283	1.00 53.35		С
ATOM	494		GLU		65	60.872	35.654	6.224	1.00 55.95		0
MOTA	495		GLU		65	59.155	35.333	7.568	1.00 54.54		0
ATOM	496	N	LYS		66	64.991	37.914	8.177	1.00 37.01		N
ATOM	497	CA	LYS		66	66.416	37.820	7.883	1.00 36.92		С
ATOM	498	C	LYS		66	67.290	38.597	8.859	1.00 34.95		C
ATOM	499	0	LYS		66	68.373	38.140	9.228	1.00 33.49		0
ATOM	500	СВ	LYS		66	66.691	38.282	6.448	1.00 38.53		C.
ATOM	501	CG	LYS		66	66.185	37.309	5.397	1.00 43.00		С
MOTA	502	CD	LYS		66	66.517	37.777	3.987	1.00 47.32		С
MOTA	503	CE	LYS		66	66.060	36.759	2.944	1.00 48.73	•	C
ATOM	504	NZ	LYS		66	66.276	37.246	1.549	1.00 49.84		N
MOTA	505	N	MET		67	66.826	39.772	9.272	1.00 33.11		N
ATOM	506	CA	MET		67	67.582	40.584	10.218	1.00 32.25		С
MOTA	507	C	MET		67	67.696	39.825	11.536	1.00.32.26	. •	С
ATOM	508	Ō	MET		67	68.780	39.717	12.106	1.00 32.78		0
ATOM	509	CB	MET		67	66.882	41.927	10.452	1.00 31.65		C
ATOM	510	CG	MET		67	67.589	42.843	11.447	1.00 30.85		С
ATOM	511	SD	MET		67	69.259	43.315	10.933	1.00 30.60		S
ATOM	512	CE	MET		67	68.905	44.374	9.529	1.00 28.51	•	С
ATOM	513	N	ALA		68	66.573	39.286	12.003	1.00 30.79		N
ATOM	514	CA	ALA		68	66.535	38.548	13.261	1.00 30.85		С
ATOM	515	C	ALA		68	67.495	37.355	13.281	1.00 31.53		С
ATOM	516	0	ALA		68	68.158	37.099	14.286	1.00 31.47		0
ATOM	517	CB	ALA		68	65.114	38.089	13.542	1.00 29.40		С
ATOM	518	N.	ILE		69	67.573	36.632	12.169	1.00 31.56		N
ATOM	519	CA	ILE		69	68.466	35.484	12.067	1.00 31.71		С
ATOM	520	C	ILE		69	69.923	35.952	12.011	1.00 31.13		C
ATOM	521	0	ILE		69	70.778	35.446	12.734	1.00 31.74		Ō
ATOM	522	CB	ILE		69	68.137	34.645	10.801	1.00 33.02		C
ATOM	523		ILE		69	66.787	33.942	10.983	1.00 34.17		C
MOTA	524		ILE		69	69.236	33.629	10.535	1.00 32.75		C
ATOM	525		ILE		69	66.173	33.422	9.680	1.00 34.42		C
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MOTA	526	N	ALA	А	70	70.194	36.933	11.155	1.00	30.92	N
ATOM	527	CA	ALA	Α	70	71.540	37.468	11.000	1.00	29.65	С
ATOM	528	C	ALA	Α	70	72.102	38.049	12.298	1.00	29.11	C
MOTA	529	0	ALA	A	70	73.278	37.866	12.602	1.00	28.78	0
ATOM	530	CB	ALA	Α	70.	71.550	38.529	9.914	1.00	30.07	C
MOTA	531	N	LEU	Α	71	71.263	38.752	13.055	1.00	28.45	N
MOTA	532	CA	LEU	A	71	71.701	39.357	14.308	1.00	28.31	C
ATOM	533	C	LEU	A	71	71.845	38.324	15.420	1.00	29.00	C
MOTA	534	0	LEU	Α	71	72.796	38.377	16.198	1.00	28.61	0
ATOM	535	CB	LEU	Α	71 .	70.726	40.453	14.742	1.00	26.49	C
MOTA	536	CG ·	LEU	Α	71	71.090	41.270	15.992	1.00	26.53	C
MOTA	537	CD1	LEU	Α	71	72.561	41.711	15.941		24.18	С
ATOM	538		LEU		71	70.168	42.487	16.073		24.70	С
ATOM	539	N	ALA	Α	72	70.899	37.392	15.502	1.00	29.36	N
ATOM	540	CA	ALA	А	72	70.966	36.355	16.526		29.89	C
MOTA	541	С	ALA		72	72.251	35.553	16.336		30.74	C
ATOM	542	0	ALA		72	72.890	35.147	17.308		29.87	0
ATOM	543	СВ	ALA		72	69.747	35.429	16.435		28.97	C
MOTA	544	N	ARG		73	72.623	35.330	15.077		31.36	N
ATOM	545	CA	ARG		73	73.832	34.580	14.761		33.37	C
MOTA	546	С	ARG		73	75.082	35.242	15.321		33.97	C
ATOM	547	0	ARG		73	76.062	34.562	15.616		34.69	o
ATOM	548	CB	ARG		73	73.988	34.414	13.247		34.83	C
ATOM	549	CG	ARG		73	73.071	33.373	12.630		37.24	C
ATOM	550	CD	ARG		73	73.289	33.268	11.124		40.12	C
ATOM	551	NE	ARG		73	72.462	32.222	10.531		43.25	N
ATOM	552	CZ	ARG		73	72.258	32.069	9.225		45.18	C
ATOM	553		ARG		73	72.821	32.899	8.354		44.94	N
ATOM	554		ARG		73	71.484	31.083	8.789		45.96	N
ATOM	555	N	GLU		74	75.050	36.566	15.463		33.85	N
ATOM	556	CA	GLU		74	76.198	37.293	15.403		33.08	C
ATOM	557	C	GLU		74	76.089	37.514	17.501		31.63	C
ATOM	558	0	GLU		74	77.011	38.037	18.119		32.56	0
ATOM	559	CB	GLU		74	76.367	38.642	15.286		34.18	C
ATOM	560	CG	GLU		74	76.569	38.544	13.779		37.13	C
ATOM	561	CD	GLU		74 74	77.709	37.611	13.779		39.95	C
ATOM	562	OE1			7 <del>4</del> 74						
ATOM	563	OE2	GLU			78.834	37.775 36.718	13.909		41.16	0
ATOM	564		GLY		74 75	77.478 74.964		12.539 18.095		30.42	0
ATOM	565	N CA	GLY		75 75	74.820	37.127 37.284	19.533		29.77	N C
ATOM					75 75				•		
ATOM	566 567	C	GLY GLY		75 75	73.815	38.310	20.019		29.50	C
ATOM		O				73.598	38.439	21.222		29.13	0
	568 560	N	GLY		76	73.212	39.051	19.096		29.23	N
ATOM	569 570	CA	GLY		76 76	72.226	40.042	19.483		28.60	C
ATOM	570	C	GLY		76 76	70.831	39.498	19.245		28.37	C
ATOM	571	0	GLY		76	70.668	38.304	18.976		26.97	0
ATOM	572	N	ILE		77	69.823	40.361	19.345		27.56	N
ATOM	573	CA	ILE		77	68.445	39.937	19.122		27.52	C
ATOM	574	C	ILE		77	67.643	41.025	18.409		28.94	C
ATOM	575	0	ILE		77 7 <b>7</b>	67.905	42.221	18.572		28.96	0
MOTA	576	CB	ILE		7 <b>7</b>	67.750	39.578	20.455		26.85	C
ATOM	577		ILE		77 77	66.524	38.704	20.183		27.10	C
ATOM	578		ILE		77	67.332	40.852	21.205		24.72	C
ATOM	579		ILE		77	65.800	38.268	21.443		24.29	C
ATOM	580	N	SER		78	66.674	40.602	17.605		28.99	N
ATOM	581	CA	SER		78 70	65.824	41.529	16.872		28.68	C
ATOM	582	С	SER	A	78	64.409	41.496	17.423	T.00	28.78	С

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MOTA	583	0	SER	A	78	63.950	40.469	17.913	1.00 30.10		0
MOTA	584	CB	SER	Α	78	65.775	41.160	15.387	1.00 27.58		С
ATOM	585	OG	SER	A	78	67.004	41.415	14.743	1.00 27.37		0
ATOM	586	N	PHE		79	63.727	42.632	17.357	1.00 28.40		N
ATOM	587	CA	PHE		79	62.350	42.710	17.807	1.00 28.34		C
ATOM	588	C	PHE		79	61.494	42.893	16.558	1.00 28.91		С
		0	PHE		79	61.360	44.004	16.048	1.00 29.07		0
ATOM	589					62.150	43.885	18.778	1.00 26.91		C
ATOM	590	CB	PHE		79			20.155	1.00 27.54		C
ATOM	591	CG	PHE		79	62.715	43.635				C
ATOM	592		PHE		79	64.067	43.839	20.421	1.00 28.32		C
ATOM	593		PHE		79	61.902	43.146	21.175	1.00 27.29		
MOTA	594		PHE		79	64.601	43.555	21.685	1.00 28.62		C
MOTA	595	CE2	PHE	Α	79	62.426	42.861	22.436	1.00 27.31		C
ATOM	596	CZ	PHE	A	79	63.7 <b>7</b> 5	43.065	22.691	1.00 27.27		С
MOTA	597	N	ILE	Α	80	60.947	41.789	16.053	1.00 28.75		N
ATOM	598	CA	ILE	Α	80	60.102	41.815	14.861	1.00 29.29		C
ATOM	599	С	ILE		80	59.054	42.919	15.011	1.00 29.89		C
ATOM	600	0	ILE		80	58.319	42.950	16.000	1.00 30.34		0
ATOM	601	CB	ILE		80	59.384	40.450	14.657	1.00 29.92		C
	602	CG1	ILE		80	60.416	39.326	14.516	1.00 30.32		С
ATOM							40.498	13.414	1.00 29.91		C
ATOM	603		ILE		80	58.499		13.341	1.00 30.51		C
ATOM	604		ILE		80	61.356	39.496		1.00 30.31		N
ATOM	605	N	PHE		81	58.981	43.821	14.035			C
MOTA	606	CA	PHE		81	58.027	44.922	14.120	1.00 31.72		
MOTA	607	С	PHE		81	56.579	44.473	14.289	1.00 31.73		C
ATOM	608	0	PHE	А	81	56.136	43.510	13.661	1.00 32.24		0
MOTA	609	CB	PHE	Α	81	58.150	45.861	12.905	1.00 32.72		С
MOTA	610	CG	PHE	Α	81	57.886	45.203	11.573	1.00 34.52		С
ATOM	611	CD1	PHE	A	81	58.857	44.422	10.959	1.00 34.19		C
ATOM	612	CD2	PHE	A	81	56.673	45.396	10.918	1.00 35.24		C
ATOM	613		PHE		81	58.625	43.844	9.708	1.00 34.16		С
ATOM	614		PHE		81	56.432	44.823	9.668	1.00 35.18		С
ATOM	615	CZ	PHE		81	57.410	44.048	9.064	1.00 34.69		C
MOTA	616	N	GLY		82	55.851	45.179	15.152	1.00 31.39		N
			GLY		82	54.462	44.851	15.401	1.00 32.43		C
ATOM	617	CA				53.490	45.673	14.574	1.00 33.20		C
MOTA	618	C	GLY		82				1.00 33.41		Ö
MOTA	619	0	GLY		82	52.277	45.505	14.688			N
MOTA	620	N	SER		83	54.012	46.567	13.741	1.00 33.11		C
ATOM	621	CA	SER		83	53.156	47.392	12.900	1.00 34.17		C
MOTA	622	C	SER		83	52.759	46.625	11.640	1.00 34.38		
ATOM	623	0	SER	Α	83	53.044	47.038	10.517	1.00 34.03	•	0
MOTA	624	CB	SER	Α	83	53.867	48.697	12.534	1.00 33.42		C
MOTA	625	OG	SER	Α	83	55.143	48.439	11.990	1.00 34.18		0
ATOM	626	N	GLN	A	84	52.110	45.487	11.855	1.00 35.41		N
ATOM	627	CA	GLN	A	84	51.640	44.625	10.780	1.00 36.62		C
ATOM	628	C	GLN		84	50.585	43.711	11.397	1.00 37.53		C
MOTA	629	0	GLN		84	50.373	43.741	12.611	1.00 36.60		0
ATOM	630	СВ	GLN		84	52.794	43.797	10.201	1.00 37.29		С
ATOM	631	CG	GLN		84	53.412	42.805	11.174	1.00 37.90		С
			GLN		84	54.568	42.035	10.563	1.00 39.55		С
MOTA	632	CD				54.427	41.416	9.510	1.00 41.11		Ō
MOTA	633		GLN		84		42.065	11.228	1.00 41.11		N
ATOM	634		GLN		84	55.720			1.00 39.70		N
ATOM	635	N	SER		85	49.921	42.908	10.571			C
ATOM	636	CA	SER		85	48.888	42.013	11.079	1.00 40.37		C
MOTA	637	С	SER		85	49.485	41.050	12.092	1.00 40.61		
MOTA	638	0	SER		85	50.655	40.678	11.993	1.00 40.59		0
MOTA	639	CB	SER	Α	85	48.249	41.211	9.943	1.00 40.55		С

MOTA	640	OG	SER	Α	85	49.115	40.182	9.501	1.00	41.70		0
MOTA	641	N	ILE	A	86	48.667	40.657	13.063	1.00	40.88		N
ATOM	642	CA	ILE	A	86	49.079	39.732	14.108	1.00	41.21		C
MOTA	643	C	ILE	A	86 .	49.589	38.424	13.508	1.00	42.63	•	C
MOTA	644	0	ILE	A	86	50.578	37.858	13.977	1.00	42.00		0
MOTA	645	CB	ILE	A	86	47.899	39.429	15.061	1.00	40.49		С
ATOM	646	CG1			86	47.454	40.722	15.750		39.68		С
ATOM	647	CG2	ILE		86	48.299	38.366	16.079		39.80		С
ATOM	648	CD1	ILE		86	46.272	40.558	16.686		38.99		С
ATOM	649	N	GLU		87	48.918	37.952	12.462		43.90		N
MOTA	650	CA	GLU		87	49.314	36.709	11.814		45.61		С
MOTA	651	C	GLU		87	50.604	36.839	11.009		44.76		С
ATOM	652	0	GLU		87	51.355	35.874	10.879		45.04		0
ATOM	653	CB	GLU		87	48.177	36.173	10.924		47.51		С
ATOM	654	CG	GLU		87	47.243	37.229	10.324		51.63		C
MOTA	655	CD	GLU		87	46.341	37.895	11.362		53.09		C
MOTA	656	OE1	GLU		87	45.804	37.180	12.238		54.09		0
MOTA	657	OE2	GLU		87	46.156	39.131	11.290		53.94		0
MOTA	658	N	SER		88	50.865	38.025	10.470		44.57		N
MOTA	659	CA	SER		88	52.091	38.246	9.704		44.09		C
MOTA	660	C	SER		88	53.295	38.287	10.643		42.16		С
ATOM	661	0	SER		88	54.343	37.720	10.346		41.66		0
MOTA	662	CB	SER		88	52.017	39.560	8.925		45.33		С
MOTA	663	OG	SER		88	51.076	39.473	7.875		49.27		0
MOTA	664	N	GLN		89	53.137	38.966	11.774		40.30		N
MOTA	665	CA	GLN		89	54.214	39.070	12.750		39.20		С
MOTA	666	C	GLN		89	54.529	37.696	13.336		38.78		C
MOTA	667	0	GLN		89	55.695	37.325	13.477		38.47		0
ATOM	668	CB	GLN		89	53.827	40.046	13.867		37.90		C
MOTA	669	CG	GLN		89	54.856	40.158	14.984		36.29		С
ATOM	670	CD	GLN		89	54.484	41.196	16.025		35.77		С
MOTA	671		GLN		89	53.314	41.342	16.381		34.41		0
MOTA	672	NE2	GLN		89	55.483	41.910	16.534		34.88		N
MOTA	673	N	ALA		90	53.487	36.940	13.668		38.89		N
ATOM	674	CA	ALA		90	53.665	35.606	14.236		38.52		С
ATOM	675	C	ALA		90	54.416	34.706	13.258		37.75		C
MOTA	676	0	ALA		90	55.284	33.932	13.658		37.34		, 0
MOTA	677	CB	ALA		90	52.310	34.996	14.580		38.78		С
MOTA	678	N	ALA		91	54.086	34.815	11.976		37.31		N
MOTA	679	CA	ALA		91	54.751	34.007	10.960		37.66		С
ATOM	680	C	ALA			56.259	34.272	10.972		37.59	4	C
MOTA	681	0	ALA		91	57.061		10.934		37.08		0
ATOM	682	СВ	ALA		91 .	54.170	34.312	9.582		36.97		· C
ATOM	683	N	MET		92	56.644	35.544	11.023		38.21		N
ATOM	684	CA	MET		92	58.063	35.898	11.052		38.30		C.
MOTA	685	C	MET		92	58.747	35.311	12.282		37.53		C
ATOM	686	0	MET		92	59.841	34.756	12.188		37.70		0
ATOM	687	CB	MET		92	58.242	37.418	11.054		39,02		C
ATOM	688	CG	MET		92	57.888	38.093	9.747		39.39		C
ATOM	689	SD	MET		92	58.282	39.850	9.772		39.06		S
ATOM	690	CE	MET		92	57.340	40.410	8.355		38.06		C
ATOM	691	N	VAL		93	58.099	35.443	13.436		37.33		N
ATOM	692	CA	VAL		93	58.647	34.919	14.679		37.59		C
ATOM	693	C	VAL		93	58.822	33.416	14.558		38.75		C
ATOM	694	0	VAL		93	59.865	32.871	14.915		39.48		0
ATOM	695	CB	VAL		93	57.718	35.218	15.877		37.43		C
ATOM	696	CGI	VAL	A	93	58.182	34.447	17.106	1.00	35.94		С

MOTA	697	CG2	VAL	A	93	57.705	36.711	16.162	1.00	36.07		C
ATOM	698	N	HIS	A	94	57.795	32.749	14.042	1.00	40.16		N
ATOM	699	CA	$\mathtt{HIS}$	A	94	57.833	31.301	13.875	1.00	40.66		С
MOTA	700	С	HIS	A	94	58.930	30.881	12.898	1.00	40.13		C
MOTA	701	0	HIS	A	94	59.624	29.888	13.122	1.00	40.44		0
MOTA	702	CB	HIS	А	94	56.466	30.797	13.395	1.00	42.53		C
ATOM	703	CG	HIS	A	94	56.400	.29.312	13.209	1.00	43.62		С
MOTA	704	NDl	HIS	A	94	56.844	28.683	12.065	1.00	44.37		N
ATOM	705		HIS		94	55.961	28.331	14.033	1.00	43.39		С
MOTA	706	CE1	HIS	Α	94	56.680	27.379	12.191	1.00	44.17		C
ATOM	707	NE2			94	56.146	27.139	13.376	1.00	44.00		N
ATOM	708	N	ALA		95	59.092	31.642	11.821	1.00	39.31		N
ATOM ·	709	CA	ALA		95	60.111	31.335	10.825		38.23		С
ATOM	710	C	ALA		95	61.516	31.408	11.425		38.43		C
ATOM	711	Ō	ALA		95	62.399	30.637	11.055		38.01		0
ATOM	712	СВ	ALA		95	59.996	32.298	9.647		37.20		C
ATOM	713	N	VAL		96	61.720	32.341	12.350		38.46		N
ATOM	714	CA	VAL		96	63.019	32.504	12.992		37.77		C
ATOM	715	C	VAL		96	63.293	31.366	13.973		38.35		Ċ
ATOM	716	0	VAL		96	64.383	30.794	13.983		37.59		Ö
ATOM		CB	VAL.		96	63.103	33.858	13.748		37.72	,	C
ATOM	718		VAL		96	64.417	33.959	14.509		36.02		C
ATOM	719	CG2	VAL		96	62.985	35.009	12.757		36.81		C
ATOM	720	N	LYS		97	62.295	31.040	14.787		38.94		N
ATOM	721	CA	LYS		97	62.426	29.978	15.777		40.76		C
ATOM .	722	C	LYS		97	62.607	28.599	15.145		42.67		C
ATOM	723	0	LYS		97		27.710	15.747		43.04		0
ATOM	724				97	63.211				39.98		C
		CB	LYS			61.199	29.955	16.697				C
ATOM	725	CG	LYS		97	60.989	31.227	17.516		39.03		
ATOM	726	CD	LYS		97	62.189	31.543	18.411		37.55		C
MOTA	727	CE	LYS		97	62.416	30.474	19.472		36.48		
	728	NZ	LYS		97	63.663	30.739	20.249		34.18		N
MOTA	729	N	ASN		98	62.091	28.425	13.933		44.43		И
ATOM	730	CA	ASN		98	62.190	27.142	13.247		46.61		C
ATOM	731	C	ASN		98	63.069	27.188	12.005		46.93		C
ATOM	732	0	ASN		98	62.847	26.431	11.059		48.02		0
ATOM	733	CB	ASN		98	60.790	26.656	12.866		48.75		C
ATOM	734	CG	ASN		98	59.921	26.378	14.078		51.25		C
ATOM	735		ASN		98	58.697	26.390	13.992		53.69		0
ATOM	736		ASN		98	60.555	26.114	15.214	1.00			N
ATOM	737.		PHE		99	64.073	28.060	12.007		46.26		N
ATOM	738	CA	PHE		99	64.958	28.182	10.855		46.28		C
ATOM	739	C	PHE		99	65.891	26.987	10.674		46.62		C
ATOM	740	0	PHE		99	66.232	26.634	9.548		46.35		0
MOTA	741	CB	PHE		99	65.799	29.459	10.952		45.12		C
ATOM	742	CG	PHE		99	66.577	29.765	9.699		44.39		C
MOTA	743		PHE		99	65.918	30.122	8.526		44.53		C
MOTA	744		PHE		99	67.964	29.690	9.689		43.94		C
ATOM	745		PHE		99	66.630	30.401	7.362		44.09		C
ATOM	746		PHE		99	68.685	29.966	8.529		43.84		C
ATOM	747	CZ	PHE		99	68.018	30.323	7.365		44.07		C
ATOM	748	N	LYS			66.303	26.368	11.775		47.68		N
MOTA	749	CA	LYS			67.214	25.226	11.708		49.23		С
MOTA	750	C	LYS			66.519	23.882	11.499		50.54		C
ATOM	751	0	LYS			67.165	22.834	11.564		50.71		0
MOTA	752	CB	LYS			68.059	25.146	12.980		48.77		С
MOTA	753	CG	LYS	A	100	68.932	26.364	13.239	1.00	47.96		С

ATOM 754 CD LYS A 100 69.709 26.180 14.526 1.00 46.23 CC ATOM 755 CE LYS A 100 71.62 27.057 16.006 1.00 43.46 N N ATOM 757 N ALA A 101 65.212 23.909 11.253 1.00 51.61 N A ATOM 758 CA ALA A 101 64.447 22.683 11.040 1.00 52.22 C C ATOM 759 C ALA A 101 64.447 22.683 11.040 1.00 52.22 C C ATOM 750 C ALA A 101 64.447 22.683 11.040 1.00 52.22 C C ATOM 750 C ALA A 101 64.955 1.911 9.835 1.00 52.77 C ATOM 761 CB ALA A 101 64.961 22.412 8.711 1.00 53.93 C ATOM 761 CB ALA A 101 64.961 22.412 8.711 1.00 53.93 C ATOM 762 N HIS A 222 79.850 30.811 17.181 1.00 61.95 C ATOM 763 CA HIS A 222 79.850 30.811 17.181 1.00 61.95 C ATOM 764 C HIS A 222 79.850 30.811 17.181 1.00 61.95 C ATOM 766 CB HIS A 222 79.357 31.019 19.526 1.00 60.99 C ATOM 766 CB HIS A 222 79.357 31.019 19.526 1.00 60.99 C ATOM 766 CB HIS A 222 78.978 29.493 15.179 1.00 67.13 C ATOM 766 CB HIS A 222 78.978 29.493 15.179 1.00 67.13 C ATOM 766 CB HIS A 222 78.978 29.493 15.179 1.00 67.13 C ATOM 767 CG HIS A 222 78.986 28.202 13.656 1.00 68.00 N ATOM 767 CG HIS A 222 79.896 28.202 13.656 1.00 68.00 N ATOM 767 CG HIS A 222 79.896 28.202 13.656 1.00 68.36 N ATOM 767 CG LHIS A 222 79.896 28.202 13.656 1.00 68.36 N ATOM 767 CG LHIS A 222 79.896 28.202 13.656 1.00 68.36 N ATOM 767 CG LHIS A 222 79.896 28.202 13.656 1.00 68.36 N ATOM 770 CEI HIS A 222 79.896 28.202 13.656 1.00 68.36 N ATOM 770 CEI HIS A 222 79.896 28.202 13.656 1.00 68.36 N ATOM 770 CEI HIS A 223 76.882 33.737 1.91 19.30 50.595 C ATOM 771 NE2 HIS A 223 76.882 33.737 1.91 19.30 50.595 C ATOM 773 CA ASN A 223 76.882 33.737 1.91 19.30 50.595 C ATOM 774 C ASN A 223 76.882 33.737 1.91 19.31 1.00 50.53 C C ATOM 778 CD ASN A 223 76.882 33.737 1.91 19.31 1.00 50.53 C C ATOM 778 CD ASN A 223 76.882 33.737 1.91 19.31 1.00 50.53 C C ATOM 778 CD ASN A 223 76.882 33.737 1.91 19.31 1.00 50.53 C C ATOM 778 CD ASN A 223 76.883 33.797 19.39 1.00 55.72 C C ATOM 778 CD ASN A 223 76.883 33.797 19.39 1.00 55.72 C C ATOM 778 CD ASN A 223 76.893 34.746 19.939 1.00 55.72 C C ATOM 778 CD ASN A 223 76.893 34.746 19.939 1.00 57.5					_							_
ATOM 756 NZ LYS A 100	ATOM	754	CD	LYS	А	100	69.709	26.180	14.526	1.00	46.23	C
ATOM 756 CA ALA A 101 65.212 23.909 11.253 1.00 51.61 N ACTOM 759 C ALA A 101 64.947 21.911 9.835 1.00 52.72 C ATOM 750 O ALA A 101 64.961 22.412 8.711 1.00 53.93 O D ATOM 761 CB ALA A 101 64.961 22.412 8.711 1.00 53.93 O D ATOM 761 CB ALA A 101 64.961 22.412 8.711 1.00 53.93 O D ATOM 761 CB ALA A 101 62.974 23.011 10.40 1.00 52.31 C ATOM 762 N HIS A 222 80.602 29.634 17.602 1.00 62.86 N ATOM 763 CA HIS A 222 79.850 30.811 17.811 1.00 61.95 C ATOM 765 C HIS A 222 79.850 30.811 17.811 1.00 60.27 C C ATOM 765 C HIS A 222 79.850 30.811 17.811 1.00 60.27 C C ATOM 765 C HIS A 222 79.357 31.056 18.415 1.00 60.27 C C ATOM 765 C HIS A 222 78.960 30.402 16.323 1.00 64.41 C C ATOM 766 C B HIS A 222 78.960 30.402 16.323 1.00 64.41 C C ATOM 767 C HIS A 222 78.961 28.946 14.729 1.00 68.21 C C ATOM 768 ND HIS A 222 78.916 28.946 14.729 1.00 68.21 C C ATOM 768 ND HIS A 222 80.165 29.019 14.729 1.00 68.21 C C ATOM 767 C B HIS A 222 79.896 28.202 13.656 1.00 68.36 C C ATOM 771 NEZ HIS A 222 79.896 28.202 13.656 1.00 68.33 N ATOM 772 N ANN A 223 78.915 23.796 18.202 10.05 57.17 N ATOM 775 C ANN A 223 76.882 37.793 34.960 19.388 1.00 57.17 N ATOM 775 C ANN A 223 76.882 37.496 19.493 1.00 53.95 C C ATOM 775 C ANN A 223 76.882 31.496 19.493 1.00 55.72 C C ATOM 775 C ANN A 223 76.882 31.496 19.493 1.00 55.72 C C ATOM 775 C ANN A 223 76.882 31.496 19.493 1.00 55.72 C C ATOM 775 C ANN A 223 76.882 31.496 19.493 1.00 55.72 C C ATOM 775 C ANN A 223 76.882 31.496 19.493 1.00 55.70 N ATOM 775 C ANN A 223 76.882 31.496 19.493 1.00 55.70 N ATOM 775 C ANN A 223 76.882 31.496 19.493 1.00 55.70 N ATOM 775 C ANN A 223 76.882 31.496 19.493 1.00 55.70 N ATOM 775 C ANN A 223 81.380 34.960 19.388 1.00 48.94 C ATOM 780 D ANN A 223 81.380 34.960 19.388 1.00 48.94 C ATOM 780 D ANN A 223 81.380 34.960 19.388 1.00 48.94 C ATOM 780 D ANN A 223 81.380 34.960 19.388 1.00 48.99 D O ATOM 780 D ANN A 223 81.380 34.960 19.388 1.00 48.99 D O ATOM 780 D ANN A 223 81.380 34.960 19.388 1.00 48.99 D O ATOM 780 D ANN A 223 81.380 34.960 19.388 1.00 48.99 D O ATOM 78	MOTA	755	CE	LYS	A	100	70.672	27.320	14.777	1.00	44.66	C
ATOM 758 CA ALA A 101 64.477 22.683 11.040 1.00 52.22 C ATOM 760 0 ALA A 101 64.975 21.911 9.855 1.00 52.77 C ATOM 760 0 ALA A 101 64.976 21.911 9.855 1.00 52.31 C ATOM 761 CB ALA A 101 62.974 23.011 10.840 1.00 52.31 C ATOM 762 N HIS A 222 79.850 30.811 17.181 1.00 61.95 C ATOM 763 CA HIS A 222 79.850 30.811 17.181 1.00 61.95 C ATOM 763 CA HIS A 222 79.850 30.811 17.181 1.00 61.95 C ATOM 766 C HIS A 222 79.857 31.019 19.526 1.00 60.27 C ATOM 766 CB HIS A 222 79.357 31.019 19.526 1.00 60.09 C ATOM 766 CB HIS A 222 78.8642 30.402 16.323 1.00 60.09 C ATOM 767 CB HIS A 222 78.978 29.499 15.179 1.00 67.13 C ATOM 767 CB HIS A 222 78.9147 31.019 19.526 1.00 67.13 C ATOM 767 CB HIS A 222 78.914 28.948 14.357 1.00 68.00 N ATOM 767 CB HIS A 222 78.916 29.099 14.729 1.00 68.21 C ATOM 770 CEI HIS A 222 78.916 28.0165 29.019 14.729 1.00 68.21 C ATOM 771 NE2 HIS A 222 78.956 28.202 13.656 1.00 68.03 N ATOM 773 CA ASN A 223 78.915 28.177 13.452 1.00 68.83 N ATOM 773 CA ASN A 223 78.915 32.796 18.201 10.00 57.17 N ATOM 774 C ASN A 223 76.823 33.737 19.113 1.00 57.53 C ATOM 771 CC ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 777 C ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 777 C ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 777 C ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 778 CD ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 778 CD ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 778 CD ASN A 223 80.463 34.895 19.899 10.00 57.65 C C ATOM 779 CD ASN A 223 80.463 34.895 19.899 10.00 57.65 C C ATOM 779 CD ASN A 223 80.453 34.895 19.899 10.00 57.65 C C ATOM 779 CD ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 779 CD ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C A ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C A ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C A ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C A ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C C ASN A 223 80.450 32.795 19.548 10.00 44.21 C C ATOM 780 C C ASN A 223 80.450 32.795 10.45	ATOM	756	NZ	LYS	A	100	71.462	27.057	16.006	1.00	43.46	N
ATOM 758 CA ALA A 101 64.477 22.683 11.040 1.00 52.22 C ATOM 760 0 ALA A 101 64.975 21.911 9.855 1.00 52.77 C ATOM 760 0 ALA A 101 64.976 21.911 9.855 1.00 52.31 C ATOM 761 CB ALA A 101 62.974 23.011 10.840 1.00 52.31 C ATOM 762 N HIS A 222 79.850 30.811 17.181 1.00 61.95 C ATOM 763 CA HIS A 222 79.850 30.811 17.181 1.00 61.95 C ATOM 763 CA HIS A 222 79.850 30.811 17.181 1.00 61.95 C ATOM 766 C HIS A 222 79.857 31.019 19.526 1.00 60.27 C ATOM 766 CB HIS A 222 79.357 31.019 19.526 1.00 60.09 C ATOM 766 CB HIS A 222 78.8642 30.402 16.323 1.00 60.09 C ATOM 767 CB HIS A 222 78.978 29.499 15.179 1.00 67.13 C ATOM 767 CB HIS A 222 78.9147 31.019 19.526 1.00 67.13 C ATOM 767 CB HIS A 222 78.914 28.948 14.357 1.00 68.00 N ATOM 767 CB HIS A 222 78.916 29.099 14.729 1.00 68.21 C ATOM 770 CEI HIS A 222 78.916 28.0165 29.019 14.729 1.00 68.21 C ATOM 771 NE2 HIS A 222 78.956 28.202 13.656 1.00 68.03 N ATOM 773 CA ASN A 223 78.915 28.177 13.452 1.00 68.83 N ATOM 773 CA ASN A 223 78.915 32.796 18.201 10.00 57.17 N ATOM 774 C ASN A 223 76.823 33.737 19.113 1.00 57.53 C ATOM 771 CC ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 777 C ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 777 C ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 777 C ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 778 CD ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 778 CD ASN A 223 76.823 34.746 19.493 10.00 57.55 C ATOM 778 CD ASN A 223 80.463 34.895 19.899 10.00 57.65 C C ATOM 779 CD ASN A 223 80.463 34.895 19.899 10.00 57.65 C C ATOM 779 CD ASN A 223 80.453 34.895 19.899 10.00 57.65 C C ATOM 779 CD ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 779 CD ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C A ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C A ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C A ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C A ASN A 223 80.450 34.895 19.899 10.00 57.65 C C ATOM 780 C C ASN A 223 80.450 32.795 19.548 10.00 44.21 C C ATOM 780 C C ASN A 223 80.450 32.795 10.45	ATOM	757	N	ALA	Α	101	65.212	23.909	11.253	1.00	51.61	N
ATOM 759 C ALA A 101 64.975 21.911 9.835 1.00 52.77 C C ALA A 101 64.961 22.412 8.711 1.00 53.93 C ATOM 761 CB ALA A 101 62.974 23.011 10.840 1.00 52.31 C ATOM 761 CB ALA A 101 62.974 23.011 10.840 1.00 52.31 C ATOM 762 N HIS A 222 79.850 30.811 17.602 1.00 62.86 N A ATOM 763 CA HIS A 222 79.850 30.811 17.602 1.00 62.96 N ATOM 764 C HIS A 222 79.850 30.811 19.526 1.00 60.09 C ATOM 765 C B HIS A 222 79.357 31.019 19.526 1.00 60.09 C ATOM 766 CB HIS A 222 78.642 30.402 16.323 1.00 64.41 C ATOM 767 CG HIS A 222 78.974 29.493 1.556 18.415 1.00 60.09 C ATOM 768 ND1 HIS A 222 78.974 29.493 15.199 1.00 64.10 67.13 C ATOM 768 ND1 HIS A 222 78.974 29.493 15.199 1.00 68.00 N ATOM 768 ND1 HIS A 222 78.974 29.493 15.199 1.00 68.00 N ATOM 768 ND1 HIS A 222 78.914 28.948 14.357 1.00 68.00 N ATOM 770 NEI HIS A 222 78.591 28.177 13.452 1.00 68.36 C ATOM 771 NEZ HIS A 222 79.896 28.202 13.656 1.00 68.83 N A ATOM 772 N ASN A 223 78.915 22.796 18.202 10.00 57.17 N ATOM 773 CA ASN A 223 76.892 33.737 19.131 1.00 50.53 C C ATOM 775 C ASN A 223 76.892 33.737 19.131 1.00 50.53 C C ATOM 775 C ASN A 223 76.893 34.960 19.493 1.00 57.65 C ATOM 777 C ASN A 223 76.893 34.960 19.493 1.00 57.65 C ATOM 778 OD ASN A 223 76.893 34.960 19.493 1.00 57.65 C ATOM 778 OD ASN A 223 76.893 34.960 19.493 1.00 57.65 C ATOM 778 OD ASN A 223 76.893 34.960 19.388 1.00 57.65 C ATOM 778 OD ASN A 223 76.293 34.796 19.493 1.00 57.65 C ATOM 778 OD ASN A 223 76.893 34.996 19.399 1.00 57.65 C ATOM 778 OD ASN A 223 79.039 34.960 19.388 1.00 57.65 C ATOM 778 OD ASN A 223 78.915 34.895 19.899 1.00 57.65 C ATOM 778 OD ASN A 223 78.915 34.895 19.899 1.00 57.65 C ATOM 778 OD ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 OD ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 OD ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 780 N GLUA 224 74.438 32.779 19.548 1.00 48.40 N ASS A 224 74.438 32.779 19.548 1.00 48.40 N ASS A 224 74.438 32.779 19.548 1.00 48.40 N ASS A 225 70.638 32.910 19.503 1.00 33.89 N ATOM 780 C G LEU A 225 70.683 32.910 19.603 1.00 33.50 N AT	ATOM	758	CA	ALA	Α	101	64.447	22.683	11.040	1.00	52.22	С
ATOM 760 O ALA A 101 64.961 22.412 8.711 1.00 53.93 O ATOM 761 CB ALA A 101 62.974 23.011 10.840 1.00 52.31 C ATOM 762 N HIS A 222 80.602 29.634 17.602 1.00 62.86 N ATOM 763 CA HIS A 222 79.347 31.556 18.415 1.00 60.27 C ATOM 765 O HIS A 222 79.347 31.556 18.415 1.00 60.27 C ATOM 765 O HIS A 222 79.347 31.556 18.415 1.00 60.27 C ATOM 765 O HIS A 222 79.347 31.556 18.415 1.00 60.27 C ATOM 765 CG HIS A 222 78.642 01.402 16.323 1.00 64.41 C ATOM 767 CG HIS A 222 78.642 01.402 16.323 1.00 64.41 C ATOM 767 CG HIS A 222 78.642 01.402 16.323 1.00 64.41 C ATOM 768 ND1 HIS A 222 78.642 01.402 16.323 1.00 68.00 N ATOM 769 CD2 HIS A 222 78.591 28.177 13.452 1.00 68.36 C ATOM 770 CEL HIS A 222 78.591 28.177 13.452 1.00 68.36 C ATOM 770 CEL HIS A 222 78.591 28.177 13.452 1.00 68.36 C ATOM 771 NEZ HIS A 222 78.591 28.107 13.452 1.00 68.36 C ATOM 772 N ASN A 223 78.591 28.107 13.452 1.00 53.95 C ATOM 773 CA ASN A 223 78.918 33.583 19.319 1.00 53.95 C ATOM 774 C ASN A 223 76.882 33.737 19.113 1.00 53.95 C ATOM 775 C ASN A 223 76.882 33.737 19.113 1.00 53.95 C ATOM 775 C ASN A 223 76.882 33.737 19.113 1.00 55.73 C ATOM 776 CB ASN A 223 76.882 33.737 19.113 1.00 55.75 C ATOM 778 CD ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 CD ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 CD ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 CD ASN A 223 80.463 34.504 19.173 1.00 59.28 C ATOM 778 CD ASN A 223 80.463 34.504 19.173 1.00 59.28 C ATOM 778 CD ASN A 223 80.463 34.504 19.173 1.00 59.28 C ATOM 788 C ADU A 224 74.843 32.740 18.248 1.00 43.68 C ATOM 785 C ADU A 224 74.843 32.740 18.248 1.00 43.68 C ATOM 786 C B ADU A 224 74.843 32.790 19.595 10.00 44.20 C ATOM 786 C B ADU A 224 74.843 32.790 19.595 10.00 44.20 C ATOM 786 C B ADU A 224 74.843 32.790 19.544 1.00 34.96 C ADU A 224 74.843 32.790 19.544 1.00 34.96 C ATOM 786 C B ADU A 224 74.843 32.790 19.544 1.00 34.96 C ATOM 787 C ADU A 225 70.685 33.681 1.00 40.674 C C ATOM 788 C ADU A 224 74.843 32.790 19.544 1.00 34.40 C ATOM 798 C ADU A 225 70.685 33.685 1.00 34.99 1.0	ATOM	759	C				64.975	21.911	9.835	1.00	52.77	С
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ATOM 772 N ASN A 223 78.915 32.796 18.220 1.00 57.17 N ATOM 773 CA ASN A 223 76.378 33.583 19.319 1.00 53.95 C ATOM 774 C ASN A 223 76.882 33.737 19.113 1.00 50.53 C ATOM 775 O ASN A 223 76.882 33.737 19.113 1.00 50.53 C ATOM 775 O ASN A 223 76.293 34.746 19.493 1.00 48.94 O ATOM 777 CG ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 777 CG ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 ODI ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 NO ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 NO ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 780 NO GLU A 224 76.275 32.723 18.505 1.00 46.60 N ATOM 780 N GLU A 224 74.843 32.740 18.248 1.00 43.68 C ATOM 781 CA GLU A 224 74.438 32.179 19.548 1.00 40.12 C ATOM 783 O GLU A 224 74.438 32.179 20.542 1.00 38.99 O ATOM 784 CB GLU A 224 74.438 32.179 20.542 1.00 38.99 O ATOM 786 CD GLU A 224 74.438 30.176 18.074 1.00 44.21 C ATOM 786 CD GLU A 224 74.123 28.981 17.454 1.00 47.84 C ATOM 787 OEI GLU A 224 74.123 28.981 17.454 1.00 44.21 C ATOM 788 OE2 GLU A 224 73.924 28.977 16.221 1.00 48.39 O ATOM 789 N LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 780 CE LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 790 CA LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 791 C LEU A 225 70.983 33.681 20.681 1.00 35.11 C ATOM 793 C B LEU A 225 70.983 33.681 20.681 1.00 34.44 C ATOM 795 CD LEU A 225 70.983 33.681 20.681 1.00 33.50 O ATOM 796 CD LEU A 225 70.983 33.681 20.681 1.00 34.44 C ATOM 797 N VAL A 226 69.853 30.635 21.169 1.00 34.23 C ATOM 798 CD LEU A 225 70.983 31.653 21.169 1.00 34.23 C ATOM 798 CD LEU A 225 70.883 30.635 21.169 1.00 34.43 C ATOM 798 CD LEU A 225 70.883 30.635 21.169 1.00 34.43 C ATOM 798 CD LEU A 225 70.883 30.635 21.169 1.00 34.43 C ATOM 798 CD LEU A 225 70.883 30.635 21.169 1.00 34.99 N ATOM 798 CD LEU A 226 70.893 31.653 21.169 1.00 34.43 C C ATOM 380 CG VAL A 226 69.853 30.197 22.491 1.00 34.23 C ATOM 380 CG VAL A 226 70.492 29.372 20.488 1.00 34.80 C ATOM 800 C VAL A 226 70.892 28.897 23.344 1.00 34.80 C ATOM 803 CG2 VAL A 226 70.492 29.7	ATOM	770	CE1	HIS	А	222	78.591	28.177	13.452	1.00	68.36	С
ATOM 773 CA ASN A 223 78.378 33.583 19.319 1.00 53.95 C ATOM 774 C ASN A 223 76.882 33.737 19.113 1.00 50.53 C ATOM 775 C ASN A 223 76.893 34.746 19.493 1.00 48.94 C ATOM 776 CB ASN A 223 79.039 34.960 19.388 1.00 55.72 C ATOM 777 CG ASN A 223 80.463 34.895 19.899 1.00 57.55 C ATOM 778 OD1 ASN A 223 80.654 35.262 21.161 1.00 59.28 C ATOM 778 DD1 ASN A 223 80.654 35.262 21.161 1.00 59.28 C ATOM 780 N GLU A 224 76.275 32.723 18.505 1.00 46.60 N ATOM 781 CA GLU A 224 74.057 32.795 19.548 1.00 43.68 C ATOM 782 C GLU A 224 74.433 32.179 20.542 1.00 38.99 O ATOM 783 C G GLU A 224 74.438 32.179 20.542 1.00 44.21 C ATOM 784 CB GLU A 224 74.438 30.176 18.074 1.00 44.21 C ATOM 786 CD GLU A 224 74.834 30.176 18.074 1.00 44.21 C ATOM 787 CD1 GLU A 224 74.123 28.981 17.454 1.00 47.84 C ATOM 788 OE2 GLU A 224 74.123 28.981 17.454 1.00 48.39 O ATOM 788 OE2 GLU A 224 73.775 28.041 18.199 1.00 38.26 O ATOM 789 N LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 780 CE LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 790 CA LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 791 C LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 792 C LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 793 CB LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 794 CG LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 797 CA LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 798 CD LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 799 C LEU A 225 70.088 32.910 19.603 1.00 34.33 C ATOM 799 C LEU A 225 70.088 32.910 19.603 1.00 34.33 C ATOM 797 N VAL A 226 69.853 30.635 21.169 1.00 37.35 C ATOM 798 CD LEU A 225 70.689 31.653 21.292 1.00 34.99 N ATOM 799 CA LEU A 225 70.689 31.653 21.292 1.00 34.99 N ATOM 799 C A LEU A 225 70.492 32.794 22.491 1.00 34.33 C ATOM 800 C VAL A 226 69.853 30.635 21.169 1.00 35.80 C ATOM 801 CB VAL A 226 69.853 30.635 21.169 1.00 34.39 C ATOM 802 CG1 VAL A 226 69.853 30.635 21.325 1.00 34.39 C ATOM 803 CG2 VAL A 226 69.853 30.635 21.325 1.00 34.39 C ATOM 804 N ASP A 227 668.841 27.322 23.842 1.00 39.48 C ATOM 805 CA ASP A 227 668.841 27	ATOM	771	NE2	HIS	A	222	79.896	28.202	13.656	1.00	68.83	N
ATOM 773 CA ASN A 223 78.378 33.583 19.319 1.00 53.95 C ATOM 774 C ASN A 223 76.882 33.737 19.113 1.00 50.53 C ATOM 775 C ASN A 223 76.893 34.746 19.493 1.00 48.94 C ATOM 776 CB ASN A 223 79.039 34.960 19.388 1.00 55.72 C ATOM 777 CG ASN A 223 80.463 34.895 19.899 1.00 57.55 C ATOM 778 OD1 ASN A 223 80.654 35.262 21.161 1.00 59.28 C ATOM 778 DD1 ASN A 223 80.654 35.262 21.161 1.00 59.28 C ATOM 780 N GLU A 224 76.275 32.723 18.505 1.00 46.60 N ATOM 781 CA GLU A 224 74.057 32.795 19.548 1.00 43.68 C ATOM 782 C GLU A 224 74.433 32.179 20.542 1.00 38.99 O ATOM 783 C G GLU A 224 74.438 32.179 20.542 1.00 44.21 C ATOM 784 CB GLU A 224 74.438 30.176 18.074 1.00 44.21 C ATOM 786 CD GLU A 224 74.834 30.176 18.074 1.00 44.21 C ATOM 787 CD1 GLU A 224 74.123 28.981 17.454 1.00 47.84 C ATOM 788 OE2 GLU A 224 74.123 28.981 17.454 1.00 48.39 O ATOM 788 OE2 GLU A 224 73.775 28.041 18.199 1.00 38.26 O ATOM 789 N LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 780 CE LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 790 CA LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 791 C LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 792 C LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 793 CB LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 794 CG LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 797 CA LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 798 CD LEU A 225 70.088 32.910 19.603 1.00 34.44 C ATOM 799 C LEU A 225 70.088 32.910 19.603 1.00 34.33 C ATOM 799 C LEU A 225 70.088 32.910 19.603 1.00 34.33 C ATOM 797 N VAL A 226 69.853 30.635 21.169 1.00 37.35 C ATOM 798 CD LEU A 225 70.689 31.653 21.292 1.00 34.99 N ATOM 799 CA LEU A 225 70.689 31.653 21.292 1.00 34.99 N ATOM 799 C A LEU A 225 70.492 32.794 22.491 1.00 34.33 C ATOM 800 C VAL A 226 69.853 30.635 21.169 1.00 35.80 C ATOM 801 CB VAL A 226 69.853 30.635 21.169 1.00 34.39 C ATOM 802 CG1 VAL A 226 69.853 30.635 21.325 1.00 34.39 C ATOM 803 CG2 VAL A 226 69.853 30.635 21.325 1.00 34.39 C ATOM 804 N ASP A 227 668.841 27.322 23.842 1.00 39.48 C ATOM 805 CA ASP A 227 668.841 27	ATOM	772	N	ASN	Α	223	78.915	32.796	18.220	1.00	57.17	N
ATOM 774 C ASN A 223 76.882 33.737 19.113 1.00 50.53 C ATOM 775 O ASN A 223 76.882 33.737 19.113 1.00 50.53 C ATOM 776 CB ASN A 223 76.293 34.746 19.493 1.00 48.94 O ATOM 776 CG ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 OD1 ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 OD1 ASN A 223 80.463 34.895 19.899 1.00 57.65 C ATOM 778 ND2 ASN A 223 80.654 35.262 21.161 1.00 57.30 N ATOM 780 N GLU A 224 76.275 32.723 18.505 1.00 46.60 N ATOM 781 CA GLU A 224 74.843 32.740 18.248 1.00 43.68 C ATOM 781 CA GLU A 224 74.843 32.740 18.248 1.00 43.68 C ATOM 782 C GLU A 224 74.438 32.740 18.248 1.00 40.12 C ATOM 783 O GLU A 224 74.438 32.179 20.542 1.00 38.99 O ATOM 784 CB GLU A 224 74.419 31.502 17.449 1.00 44.21 C ATOM 785 CG GLU A 224 74.419 31.502 17.449 1.00 44.21 C ATOM 786 CD GLU A 224 74.419 31.502 17.449 1.00 44.21 C ATOM 786 CD GLU A 224 74.419 31.502 17.449 1.00 44.21 C ATOM 788 OE2 GLU A 224 74.123 28.981 17.454 1.00 47.84 C ATOM 788 OE2 GLU A 224 73.775 28.041 18.199 1.00 48.39 O ATOM 788 OE2 GLU A 224 73.775 28.041 18.199 1.00 48.39 O ATOM 789 N LEU A 225 72.962 33.546 19.527 1.00 33.83 C ATOM 791 C LEU A 225 70.932 32.704 20.479 1.00 33.51 C ATOM 792 C LEU A 225 70.932 32.704 20.479 1.00 34.43 C ATOM 793 C LEU A 225 70.932 32.704 20.479 1.00 33.83 C ATOM 794 CG LEU A 225 70.675 35.448 21.979 1.00 34.33 C ATOM 795 CD LEU A 225 70.676 35.448 21.979 1.00 34.33 C ATOM 796 CD2 LEU A 225 70.676 35.448 21.979 1.00 34.33 C ATOM 797 C LEU A 225 70.676 35.448 21.979 1.00 34.33 C ATOM 797 C LEU A 225 70.676 35.448 21.979 1.00 34.33 C ATOM 797 C LEU A 225 70.676 35.448 21.979 1.00 34.33 C ATOM 797 C LEU A 225 70.676 35.448 21.979 1.00 34.33 C ATOM 797 C LEU A 225 70.676 35.448 21.979 1.00 34.33 C ATOM 797 C LEU A 225 70.676 35.448 21.979 1.00 34.33 C ATOM 797 C LEU A 225 70.676 35.448 21.979 1.00 34.39 C ATOM 797 C VAL A 226 69.235 30.197 22.491 1.00 37.35 C ATOM 800 C VAL A 226 69.683 30.635 21.199 21.00 34.99 N ATOM 798 C C VAL A 226 69.235 30.197 22.491 1.00 37.35 C C ATOM 800 C C ASP A 227 68.841 27.592							•					С
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ATOM 787 OE1 GLU A 224 73.924 28.977 16.221 1.00 48.39 O ATOM 788 OE2 GLU A 224 73.775 28.041 18.199 1.00 48.26 O ATOM 789 N LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 790 CA LEU A 225 72.089 33.681 20.681 1.00 35.11 C ATOM 791 C LEU A 225 70.932 32.704 20.479 1.00 34.44 C ATOM 792 O LEU A 225 70.088 32.901 19.603 1.00 33.50 O ATOM 793 CB LEU A 225 71.561 35.116 20.775 1.00 33.83 C ATOM 794 CG LEU A 225 70.675 35.448 21.979 1.00 34.33 C ATOM 795 CD1 LEU A 225 70.675 35.448 21.979 1.00 34.33 C ATOM 796 CD2 LEU A 225 70.220 36.899 21.899 1.00 34.99 N ATOM 797 N VAL A 226 70.893 31.653 21.292 1.00 34.99 N ATOM 799 C VAL A 226 69.853 30.635 21.169 1.00 35.64 C ATOM 799 C VAL A 226 69.255 30.197 22.491 1.00 34.90 O ATOM 800 O VAL A 226 69.744 30.516 23.566 1.00 38.20 O ATOM 801 CB VAL A 226 70.890 29.701 19.086 1.00 33.57 C ATOM 802 CG1 VAL A 226 70.890 29.701 19.086 1.00 33.57 C ATOM 803 CG2 VAL A 226 70.890 29.701 19.086 1.00 33.57 C ATOM 804 N ASP A 227 68.128 29.462 22.397 1.00 34.39 C ATOM 805 CA ASP A 227 66.128 29.462 22.397 1.00 39.28 C ATOM 806 C ASP A 227 66.841 27.032 23.103 1.00 39.28 C ATOM 807 O ASP A 227 66.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 66.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 66.841 27.032 23.374 1.00 39.48 O ATOM 808 CB ASP A 227 66.841 27.032 23.374 1.00 39.13 C	MOTA	785	CG	GLU	A	224	74.834	30.176	18.074	1.00	46.74	С
ATOM 787 OE1 GLU A 224 73.924 28.977 16.221 1.00 48.39 O ATOM 788 OE2 GLU A 224 73.775 28.041 18.199 1.00 48.26 O ATOM 789 N LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 790 CA LEU A 225 72.089 33.681 20.681 1.00 35.11 C ATOM 791 C LEU A 225 70.932 32.704 20.479 1.00 34.44 C ATOM 792 O LEU A 225 70.088 32.901 19.603 1.00 33.50 O ATOM 793 CB LEU A 225 71.561 35.116 20.775 1.00 33.83 C ATOM 794 CG LEU A 225 70.675 35.448 21.979 1.00 34.33 C ATOM 795 CD1 LEU A 225 70.675 35.448 21.979 1.00 34.33 C ATOM 796 CD2 LEU A 225 70.220 36.899 21.899 1.00 34.99 N ATOM 797 N VAL A 226 70.893 31.653 21.292 1.00 34.99 N ATOM 799 C VAL A 226 69.853 30.635 21.169 1.00 35.64 C ATOM 799 C VAL A 226 69.255 30.197 22.491 1.00 34.90 O ATOM 800 O VAL A 226 69.744 30.516 23.566 1.00 38.20 O ATOM 801 CB VAL A 226 70.890 29.701 19.086 1.00 33.57 C ATOM 802 CG1 VAL A 226 70.890 29.701 19.086 1.00 33.57 C ATOM 803 CG2 VAL A 226 70.890 29.701 19.086 1.00 33.57 C ATOM 804 N ASP A 227 68.128 29.462 22.397 1.00 34.39 C ATOM 805 CA ASP A 227 66.128 29.462 22.397 1.00 39.28 C ATOM 806 C ASP A 227 66.841 27.032 23.103 1.00 39.28 C ATOM 807 O ASP A 227 66.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 66.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 66.841 27.032 23.374 1.00 39.48 O ATOM 808 CB ASP A 227 66.841 27.032 23.374 1.00 39.13 C	ATOM .	786	CD	GLU	Α	224	74.123	28.981	17.454	1.00	47.84	С
ATOM 788 OE2 GLU A 224 73.775 28.041 18.199 1.00 48.26 O ATOM 789 N LEU A 225 72.962 33.546 19.527 1.00 37.30 N ATOM 790 CA LEU A 225 72.089 33.681 20.681 1.00 35.11 C ATOM 791 C LEU A 225 70.932 32.704 20.479 1.00 34.44 C ATOM 792 O LEU A 225 70.088 32.901 19.603 1.00 33.50 O ATOM 793 CB LEU A 225 71.561 35.116 20.775 1.00 33.83 C ATOM 794 CG LEU A 225 71.561 35.116 20.775 1.00 34.33 C ATOM 795 CD1 LEU A 225 71.450 35.194 23.274 1.00 34.23 C ATOM 796 CD2 LEU A 225 70.675 35.448 21.979 1.00 34.33 C ATOM 797 N VAL A 226 70.893 31.653 21.292 1.00 34.99 N ATOM 798 CA VAL A 226 69.853 30.635 21.169 1.00 35.64 C ATOM 799 C VAL A 226 69.853 30.197 22.491 1.00 37.35 C ATOM 800 O VAL A 226 69.235 30.197 22.491 1.00 37.35 C ATOM 801 CB VAL A 226 69.744 30.516 23.566 1.00 38.20 O ATOM 801 CB VAL A 226 70.890 29.701 19.086 1.00 33.57 C ATOM 802 CG1 VAL A 226 70.890 29.701 19.086 1.00 34.80 C ATOM 803 CG2 VAL A 226 71.557 28.805 21.325 1.00 34.39 C ATOM 804 N ASP A 227 68.128 29.462 22.397 1.00 34.39 C ATOM 805 CA ASP A 227 67.453 28.938 23.575 1.00 39.28 C ATOM 806 C ASP A 227 67.986 27.529 23.842 1.00 39.48 O ATOM 807 O ASP A 227 66.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 66.999 28.897 23.374 1.00 39.13 C	MOTA		OE1				73.924	28.977	16.221	1.00	48.39	
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ATOM 802 CG1 VAL A 226 70.890 29.701 19.086 1.00 33.57 C ATOM 803 CG2 VAL A 226 71.557 28.805 21.325 1.00 34.39 C ATOM 804 N ASP A 227 68.128 29.462 22.397 1.00 38.54 N ATOM 805 CA ASP A 227 67.453 28.938 23.575 1.00 39.28 C ATOM 806 C ASP A 227 67.986 27.529 23.842 1.00 40.76 C ATOM 807 O ASP A 227 68.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 65.929 28.897 23.374 1.00 39.13 C ATOM 809 CG ASP A 227 65.510 28.134 22.123 1.00 39.09 C	MOTA	800	0	VAL	Α	226	69.744	30.516	23.566	1.00	38.20	
ATOM 803 CG2 VAL A 226 71.557 28.805 21.325 1.00 34.39 C ATOM 804 N ASP A 227 68.128 29.462 22.397 1.00 38.54 N ATOM 805 CA ASP A 227 67.453 28.938 23.575 1.00 39.28 C ATOM 806 C ASP A 227 67.986 27.529 23.842 1.00 40.76 C ATOM 807 O ASP A 227 68.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 65.929 28.897 23.374 1.00 39.13 C ATOM 809 CG ASP A 227 65.510 28.134 22.123 1.00 39.09 C	MOTA	801	CB	VAL	Α	226	70.412	29.372	20.488	1.00	34.80	С
ATOM 804 N ASP A 227 68.128 29.462 22.397 1.00 38.54 N ATOM 805 CA ASP A 227 67.453 28.938 23.575 1.00 39.28 C ATOM 806 C ASP A 227 67.986 27.529 23.842 1.00 40.76 C ATOM 807 O ASP A 227 68.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 65.929 28.897 23.374 1.00 39.13 C ATOM 809 CG ASP A 227 65.510 28.134 22.123 1.00 39.09 C	MOTA	802	CG1	VAL	A	226	70.890	29.701	19.086	1.00	33.57	С
ATOM 804 N ASP A 227 68.128 29.462 22.397 1.00 38.54 N ATOM 805 CA ASP A 227 67.453 28.938 23.575 1.00 39.28 C ATOM 806 C ASP A 227 67.986 27.529 23.842 1.00 40.76 C ATOM 807 O ASP A 227 68.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 65.929 28.897 23.374 1.00 39.13 C ATOM 809 CG ASP A 227 65.510 28.134 22.123 1.00 39.09 C		803								1.00	34.39	
ATOM 805 CA ASP A 227 67.453 28.938 23.575 1.00 39.28 C ATOM 806 C ASP A 227 67.986 27.529 23.842 1.00 40.76 C ATOM 807 O ASP A 227 68.841 27.032 23.103 1.00 39.48 O ATOM 808 CB ASP A 227 65.929 28.897 23.374 1.00 39.13 C ATOM 809 CG ASP A 227 65.510 28.134 22.123 1.00 39.09 C												
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010 010 0D1 ADF A 227 00.130 27.104 21.740 1.00 39.00 U												
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ATOM	811	OD2	ASP	Α	227		64.472	28.498	21.529	1.00	38.30		0
ATOM	812	N	SER	Α	228		67.478	26.888	24.891	1.00	43.19		N
ATOM	813	CA	SER	Α	228		67.918	25.544	25.262	1.00	45.34		С
ATOM	814	С	SER	Α	228		67.723	24.504	24.157	1.00	46.69		С
ATOM	815	0	SER	Α	228		68.239	23.388	24.255	1.00	47.84		0
MOTA	816	CB	SER	A	228		67.202	25.088	26.537	1.00	45.27		С
ATOM	817	OG	SER				65.796	25.143	26.379	1.00	46.27		0
ATOM	818	N	GLN				66.988	24.868	23.110		47.37		N
ATOM	819	CA	GLN				66.746	23.962	21.990		47.48		С
ATOM	820	C	GLN				67.631	24.320	20.797		47.27		С
ATOM	821	0	GLN				67.433	23.812	19.691		46.74		0
ATOM	822	СВ	GLN				65.272	24.014	21.573		48.89		C
ATOM	823	CG			229		64.301	23.525	22.639		50.86		C
ATOM	824	ĊD	GLN				62.849	23.622	22.197		53.57		C
ATOM	825		GLN				.62.439	22.989	21.221		54.79		0
ATOM	826	NE2	GLN				62.063	24.421	22.913		54.30		N
ATOM	827	N	LYS				68.603	25.200	21.032		46.64		N
ATOM	828	CA	LYS				69.534	25.642	19.994		45.65		C
ATOM	829	C	LYS			٠	68.876	26.513	18.925		43.41		C
ATOM	830	0	LYS				69.462	26.758	17.870		43.63		0
ATOM	831	СВ	LYS				70.199	24.434	19.324		48.29		C
ATOM	832	CG	LYS				70.961	23.521	20.277		52.07		C
ATOM	833	CD	LYS				72.156	24.222	20.277		55.27		C
ATOM	834	CE				٠	72.130				57.57		C
			LYS LYS					23.286	21.871				
ATOM	835	NZ					74.090	23.919	22.492		58.56 41.68		N
ATOM	836	N	ARG				67.663	26.982	19.197				N
ATOM	837	CA	ARG				66.947	27.829	18.246		40.28		C
ATOM	838	C			231		67.277	29.302	18.488		38.35		C
ATOM	839	0	ARG				67.386	29.739	19.634		36.97		0
ATOM	840	CB	ARG				65.438	27.626	18.386		41.68		C
ATOM	841	CG	ARG				64.972	26.186	18.232		43.64		C
ATOM	842	CD			231		63.472	26.084	18.443		45.03		C
ATOM	843	NE	ARG				63.077	26.614	19.746		46.86		N
ATOM	844	CZ	ARG				61.817	26.753	20.150		48.34		C
ATOM	845		ARG				60.814	26.402	19.354		48.72		N
ATOM	846	NH2					61.559	27.248	21.355		49.43		N
ATOM	847	N			232		67.431	30.061	17.406		36.49		N
	848	CA			232		67.742	31.483	17.510		34.28		C
ATOM	849	C .			232	•	66.713	32.225	18.352		33.16		C
ATOM	850	0			232		65.514	31.959	18.265		33.82		0
ATOM	851	CB	TYR				67.791	32.131	16.127		33.26		C
MOTA	852	CG			232		68.892	31.630	15.232		32.73		C
MOTA	853		TYR				70.213	31.584	15.672		32.85		C
ATOM	854		TYR				68.614	31.215	13.932		33.54		C
ATOM	855		TYR				71.237	31.131	14.830		33.51		C
ATOM	856	CE2					69.620	30.764	13.087		33.65		C
MOTA	857	CZ			232		70.927	30.724	13.540		33.53		С
ATOM	858	OH			232		71.910	30.270	12.695		34.70		0
MOTA	859	N			233		67.186	33.151	19.177		32.10		N
ATOM	860	CA			233		66.290	33,942	20.008		31.00		C
ATOM	861	C			233		65.707	35.036	19.132		29.82		C
ATOM	862	0			233		66.346	35.479	18.175		29.69		0
ATOM	863	CB			233		67.051	34.571	21.180		30.50		C
ATOM	864	CG			233		66.828	33.952	22.564		32.28		С
MOTA	865		LEU				66.898	32.442	22.480		31.52		С
MOTA	866		LEU				67.867	34.488	23.542		30.57		C
ATOM	867	N	VAL	Α	234		64.491	35.461	19.446	1.00	28.87		N

ATOM	868	CA	VAL	<b>Z</b> \	234	63.855	36.517	18.675	1 00	28.85	C
		C	VAL				37.272	19.552			
ATOM	869					62.872				29.58	C
ATOM	870	0	VAL			62.257	36.699	20.454		29.60	0
MOTA	871	CB	VAL			63.113	35.952	17.431		28.52	С
MOTA	872	CG1	VAL	Α	234	61.924	35.100	17.861	1.00	27.33	C
ATOM	873	CG2	VAL	Α	234	62.669	37.091	16.533	1.00	26.42	С
ATOM	874	N	GLY	A	235	62.752	38.571	19.299	1.00	29.15	N
ATOM	875	CA	GLY	Α	235	61.835	39.387	20.065	1.00	29.25	С
ATOM ·	876	С	GLY			60.701	39.852	19.178		30.00	C
ATOM	877	0	GLY			60.745	39.678	17.955		29.63	ō
ATOM	878	N			236	59.680	40.444	19.786		29.18	N
ATOM	879	CA						19.023		29.42	C
			ALA			58.545	40.932				
ATOM	880	C			236	57.930	42.156	19.681		28.94	C
ATOM	881	0	ALA			57.700	42.175	20.887		30.25	0
ATOM	882	CB	ALA			57.502	39.828	18.880		30.04	C
MOTA	883	N	GLY			57.675	43.185	18.885		28.85	N
MOTA	884	CA	$\operatorname{GLY}$	Α	237	57.072	44.386	19.426	1.00	29.68	С
MOTA	885	C	GLY	Α	237	55.565	44.232	19.522	1.00	30.66	С
ATOM	886	0	GLY	A	237	54.957	43.541	18.700	1.00	31.29	0
ATOM	887	N	ILE	Α	238	54.969	44.850	20.540	1.00	30.86	N
ATOM	888	CA			238	53.524	44.811	20.734		31.71	C
ATOM	889	C			238	53.038	46.228	21.055		32.48	C
ATOM	890	0			238	53.834	47.106	21.385		31.88	Ō
	891	CB					43.869	21.901		32.49	C
MOTA			ILE			53.107					
ATOM	892	CG1	ILE			53.631	44.409	23.233		32.43	C
MOTA	893	CG2	ILE			53.626	42.458	21.652		31.98	C
ATOM	894	CD1	ILE			53.098	43.658	24.452		31.48	С
MOŢA	895	N			239	51.732	46.451	20.946	1.00	32.65	N
ATOM .	896	CA	ASN	Α	239	51.171	47.761	21.232	1.00	33.12	C
MOTA	897	C	ASN	Α	239	50.172	47.661	22.375	1.00	34.35	C
MOTA	898	0	ASN	Α.	239	49.801	46.559	22.798	1.00	34.32	0
MOTA	899	CB	ASN	Α	239	50.508	48.344	19.977	1.00	33.45	С
MOTA	900	CG	ASN			49.374	47.478	19.450	1.00	33.90	C
ATOM	901		ASN			48.333	47.342	20.090		33.39	0
ATOM	902		ASN			49.576	46.889	18.278		33.29	N
ATOM	903	N	THR			49.743	48.810	22.883		35.36	N
ATOM	904	CA	THR								C
						48.799	48.847	23.993		35.80	
ATOM	905	C	THR			47.337	48.691	23.576		37.42	C
ATOM	906	0	THR			46.444	48.870	24.401		36.13	0
MOTA	907	CB	THR			48.923	50.162	24.770		34.93	C
ATOM	908		THR			48.776	51.257	23.859		34.76	0
ATOM	909	CG2	THR	Α	240	50.273	50.252	25.467	1.00	33.70	C
MOTA	910	N	ARG	A	241	47.086	48.349	22.313	1.00	39.17	N
ATOM	911	CA	ARG	A	241	45.707	48.208	21.853	1.00	42.57	C
MOTA	912	C	ARG	Α	241	45.212	46.785	21.603	1.00	42.28	C
MOTA	913	0	ARG	Α	241	44.262	46.347	22.247	1.00	43.14	0
ATOM	914	CB	ARG			45.484	49.058	20.598	1.00	45.89	С
ATOM	915	CG	ARG			45.948	50.498	20.767		51.37	С
ATOM	916	CD			241	45.095	51.484	19.983		56.20.	C
ATOM	917	NE	ARG			45.628	52.843	20.084		60.59	N
ATOM	918	CZ			241		53.947				C
						44.928		19.834		62.98	
ATOM	919		ARG			43.654	53.862	19.468		63.64	N
ATOM	920		ARG			45.505	55.138	19.945		64.03	N
MOTA	921	N	ASP			45.843	46.063	20.682		41.72	N
ATOM	922	CA	ASP			45.410	44.698	20.373		42.47	С
ATOM	923	C	ASP	Α	242	46.241	43.591	21.030	1.00	41.62	С
MOTA	924	0	ASP	Α	242	46.326	42.488	20.501	1.00	41.70	0

ATOM	925	CB	ASP	Α	242	45.403	44.478	18.853	1.00 42.18	C
ATOM	926	CG	ASP	A	242	46.799	44.528	18.240	1.00 44.11	,C
ATOM	927	OD1	ASP	A	242	47.791	44.451	18.998	1.00 43.54	0
MOTA	928		ASP			46.903	44.631	16.995	1.00 42.81	0
ATOM	929	N			243	46.830	43.876	22.186	1.00 41.52	N
ATOM	930	CA			243	47.668	42.897	22.878	1.00 41.20	С
ATOM	931	C			243	46.966	41.623	23.352	1.00 42.11	С
ATOM	932	0			243	47.603	40.573	23.467	1.00 42.24	0
ATOM	933	СВ			243	48.387	43.565	24.058	1.00 38.57	c
ATOM	934	CG			243	47.465	44.128	25.095	1.00 37.00	Ċ
ATOM	935		PHE			46.983	43.327	26.123	1.00 36.77	C
ATOM	936		PHE			47.083	45.464	25.051	1.00 36.43	C
ATOM	937		PHE			46.136	43.847	27.096	1.00 35.68	c
ATOM	938	CE2				46.237	45.996	26.017	1.00 35.00	C
ATOM	939	CZ			243	45.762	45.185	27.044	1.00 36.83	C
ATOM	940	N			244	45.666	41.702	23.623	1.00 43.08	N
ATOM	941	CA	ARG			44.926	40.526	24.078	1.00 43.08	C
ATOM	942	CA	ARG						1.00 43.54	C
						44.890	39.447	22.996		
ATOM	943	0	ARG			44.803	38.257	23.297	1.00 43.24	0
ATOM	944	CB	ARG			43.502	40.914	24.498	1.00 43.28	C
ATOM	945	CG	ARG			43.455	41.843	25.705	1.00 43.47	C
ATOM	946	CD	ARG			42.029	42.095	26.172	1.00 44.74	C
ATOM	947	NE	ARG			41.971	43.071	27.259	1.00 45.31	N
MOTA	948	CZ			244	42.192	44.376	27.110	1.00 46.31	C
ATOM	949		ARG			42.485	44.872	25.914	1.00 44.51	N
ATOM	950		ARG			42.123	45.188	28.159	1.00 44.79	N
MOTA	951	N			245	44.960	39.867	21.736	1.00 44.04	N
ATOM	952	CA	GLU			44.959	38.928	20.618	1.00 44.49	С
ATOM	953	C	GLU			46.371	38.707	20.078	1.00 43.54	C
MOTA	954	Ο,	GLU			46.720	37.601	19.665	1.00 43.64	0
ATOM	955	CB			245	44.067	39.439	19.479	1.00.47.18	С
ATOM	956	ÇG	GLU	А	245	42.599	39.036	19.570	1.00 51.54	, С
MOTA	957	CD	GLU	A	245	41.917	39.551	20.822	1.00 54.39	C
ATOM	958	OE1				41.972	40.777	21.070	1.00 56.74	0
ATOM	959	. OE2	GLU	Α	245	41.320	38.730	21.555	1.00 56.12	0
ATOM	960	N	ARG	Α	246	47.183	39.761	20.088	1.00 41.72	, N
ATOM	961	CA	ARG	A	246	48.547	39.679	19.569	1.00 40.10	C
ATOM .	962	C	ARG	A	246	49.529	38.897	20.449	1.00 38.51	C
MOTA	963	0	ARG	Α	246	50.305	38.087	19.943	1.00 37.50	0
MOTA	964	CB	ARG	Α	246	49.093	41.091	19.314	1.00 39.02	C
ATOM	965	CG	ARG	Α	246	50.417	41.125	18.558	1.00 38.76	. C
MOTA	966	CD	ARG	Α	246	50.877	42.560	18.333	1.00 39.34	C
MOTA	967	NE	ARG	Α	246	49.978	43.314	17.460	1.00 37.43	N
ATOM	968	CZ	ARG	Α	246	49.985	43.242	16.132	1.00 38.30	C
ATOM	969	NH1	ARG	Α	246	50.847	42.450	15.507	1.00 37.21	N
ATOM	970	NH2	ARG	Α	246	49.129	43.967	15.422	1.00 39.33	N
MOTA	971	N	VAL	Α	247	49.502	39.137	21.756	1.00 37.24	N
MOTA	972	CA	VAL	Α	247	50.414	38.440	22.657	1.00 37.34	C
ATOM	973	C	VAL	Α	247	50.303	36.918	22.523	1.00 38.18	C
ATOM	974	0			247	51.292	36.251	22.209	1.00 38.12	0
ATOM	975	СВ			247	50.185	.38.872	24.129	1.00 36.77	C
ATOM	976		VAL			 51.023	38.026	25.070	1.00 35.70	C
ATOM	977		VAL			50.550	40.343	24.293	1.00 37.03	C
ATOM	978	N			248	49.100	36.347	22.747	1.00 38.57	N
ATOM	979	CA			248	48.934	34.892	22.631	1.00 38.12	C
ATOM	980	C.			248	49.506	34.329	21.333	1.00 37.59	c
ATOM	981	Ō			248	50.166	33.293	21.336	1.00 37.87	0
		-				30.100	55.25		,	J

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MOTA	982	CB	PRO	Α	248		47.422	34.714	22.729	1.00 38.80	С
ATOM	983	CG	PRO	A	248		47.039	35.791	23.701	1.00 38.59	C
MOTA	984	CD	PRO	А	248		47.840	36.979	23.188	1.00 38.38	C
MOTA	985	N	ALA	A	249		49.256	35.016	20.224	1.00 37.30	N
ATOM	986	CA	ALA				49.763	34.573	18.932	1.00 38.37	С
ATOM	987	C	ALA				51.292	34.588	18.923	1.00 39.52	С
ATOM	988	0	ALA				51.931	.33.682	18.379	1.00 38.98	0
ATOM	989	СВ	ALA				49.228	35.471	17.826	1.00 38.41	С
ATOM	990	N	LEU				51.872	35.625	19.526	1.00 39.58	N
ATOM	991	CA	LEU				53.322	35.761	19.587	1.00 39.74	С
ATOM	992	C	LEU				53.935	34.682	20.475	1.00 39.38	С
MOTA	993	0	LEU			,	54.951	34.082	20.123	1.00 38.34	0
ATOM	994	СВ	LEU			,	53.695	37.163	20.092	1.00 39.96	C
	995	CG	LEU				54.043	38.222	19.029	1.00 40.83	С
MOTA	996		LEU				53.463	37.859	17.678	1.00 39.28	C
ATOM			LEU				53.540	39.582	19.487	1.00 39.93	C
ATOM	997						53.310	34.434	21.620	1.00 39.76	Ŋ
ATOM	998	N	VAL				53.793	33.409	22.537	1.00 41.50	C
ATOM	999	CA	VAL						21.845	1.00 42.53	C
MOTA	1000	C			251		53.714	32.055		1.00 42.76	O
MOTA	1001	0	VAL				54.690	31.303	21.810	1.00 42.70	c
MOTA	1002	CB			251		52.940	33.354		1.00 41.82	C
MOTA	1003		VAL				53.352	32.161	24.671		c
MOTA	1004		VAL				53.104	34.644	24.600	1.00 41.93	N
ATOM	1005	N			252		52.541	31.756	21.293	1.00 43.62	C
MOTA	1006	CA			252		52.317	30.500	20.590	1.00 43.74	C
MOTA	1007	C			252		53.332	30.314	19.465	1.00 41.50	
MOTA	1008	0			252		53.789	29.203	19.215	1.00 41.39	0
MOTA	1009	CB			252		50.893	30.456	20.020	1.00 46.53	C
MOTA	1010	CG			252		49.920	29.576	20.810	1.00 51.69	C
MOTA	1011	CD			252		49.586	30.124	22.193	1.00 54.01	C
MOTA	1012		GLU				48.841	31.128	22.279	1.00 53.93	0
MOTA	1013	OE2	GLU	Α	252		50.070	29.545	23.194	1.00 55.79	0
MOTA	1014	N	ALA	Α	253		53.682	31.404	18.788	1.00 38.82	N
MOTA	1015	CA	ALA	Α	253		54.651	31.343	17.698	1.00 36.89	C
MOTA	1016	C	ALA	A	253		56.078	31.102	18.212	1.00 36.24	C
MOTA	1017	0			253		56.968	30.739	17.441	1.00 35.13	0
MOTA	1018	CB			253		54.596	32.622	16.881	1.00 35.91	С
MOTA	1019	N			254		56.292	31.313	19.510	1.00 35.29	N
MOTA	1020	CA	$\operatorname{GLY}$	A	254		57.609	31.085	20.086	1.00 35.95	C
MOTA	1021	C	GLY	A	254		58.480	32.301	20.380	1.00 35.64	C
ATOM	1022	0	GLY	A	254		59.684	32.159	20.578		0
ATOM	1023	N	ALA	Α	255		57.895	33.493		1.00 35.20	N
MOTA	1024	CA	ALA	A	255		58.675	34.694	20.697	1.00 33.82	С
MOTA	1025	С	ALA	Α	255		59.321	34.554	22.074	1.00 32.75	C
ATOM	1026	0	ALA	A	255		58.653	34.196	23.045	1.00 32.02	0
MOTA	1027	CB	ALA	Α	255		57.779	35.922	20.657	1.00 33.94	C
MOTA	1028	N	ASP	A	256		60.621	34.834	22.156	1.00 31.67	N
MOTA	1029	CA	ASP	Α	256		61.351	34.723	23.418	1.00 32.02	C
MOTA	1030	С	ASP	Α	256		61.145	35.912	24.355	1.00 31.11	C
MOTA	1031	0	ASP	Α	256		61.234	35.777	25.574	1.00 30.14	0
MOTA	1032	CB			256		62.841	34.541	23.139	1.00 33.02	С
ATOM	1033	CG			256		63.129	33.275	22.362	1.00 34.81	C
ATOM	1034				256		63.114	32.188		1.00 36.54	0
MOTA	1035				256		63.350			1.00 33.32	0
ATOM	1036	N			257			37.077		1.00 30.39	N
ATOM	1037	CA			257			38.271		1.00 29.66	С
ATOM	1038	C			257		59.823			1.00 29.38	C
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ATOM	1039	0	VAL	Α	257	59.879	39.308	22.582	1.00	28.28			0
MOTA	1040	CB	VAL	Α	257	62.012	38.911	24.988	1.00	29.16			C
ATOM	1041	CG1	VÄL	Α	257	62.829	39.194	23.747	1.00	29.29			C
MOTA	1042	CG2	VAL	Α	257	61.782	40.177	25.798	1.00	28.00			С
MOTA	1043	N	LEU	Α	258	59.038	40.065	24.523	1.00	28.75			N
MOTA	1044	CA	LEU	Α	258	58.187	41.059	23.886	1.00	29.85			С
MOTA	1045	С	LEU			58.608	42.453	24.344	1.00	29.91			С
ATOM	1046	0	LEU			59.381	42.597	25.293		30.16			0
ATOM	1047	СВ	LEU			56.720	40.823	24.265		28.53			C
ATOM	1048	CG	LEU			56.167	39.402	24.111		29.86			C
ATOM	1049		LEU			54.713	39.397	24.543		30.36			C
ATOM	1050		LEU			56.296	38.921	22.670		28.79			C
ATOM	1051	N			259	58.104	43.477	23.663		29.40			N
ATOM	1052	CA	CYS			58.416	44.850	24.034		28.72			C
ATOM	1053	C	CYS			57.344	45.795	23.530		27.77			C
ATOM	1054	0			259	57.043	45.820	22.337		27.16			0
ATOM	1055				259					28.20			C
		CB				59.772 60.305	45.285	23.465					s
MOTA	1056	SG			259		46.904	24.092		28.27			
ATOM	1057	N			260	56.766	46.564	24.446		28.22	٠.		N
ATOM	1058	CA			260	55.744	47.533	24.083		29.67			C
ATOM	1059	C			260	56.463	48.683	23.373		31.98			C
ATOM	1060	0			260	57.365	49.308	23.927		31.74			0
ATOM	1061	CB			260	55.010	48.056	25.325		28.89			C
ATOM	1062	CG1			260	54.391	46.877	26.086		28.30			C
MOTA	1063	CG2	ILE			53.926	49.045	24.912		26.45			C
MOTA	1064		ILE			53.791	47.257	27.423		26.77			C
ATOM	1065	N	ASP			56.045	48.936	22.139		33.17			N
MOTA	1066	CA	ASP			56.625	49.951	21.267		35.06			C
MOTA	1067	C	ASP			55.836	51.272	21.315		35.12			C
MOTA	1068	0	ASP	Α	261	54.712	51.338	20.820	1.00	36.56			0
MOTA	1069	CB	ASP	Α	261	56.647	49.349	19.852	1.00	36.45			С
MOTA	1070	CG	ASP	Α	261	57.248	50.264	18.819	1.00	38.72			C
MOTA	1071		ASP			58.086	51.109	19.176	1.00	41.12			0
ATOM	1072	OD2	ASP	А	261	56.892	50.118	17.630	1.00	41.11			0
MOTA	1073	N	SER	Α	262	56.420	52.321	21.902	1.00	33.61			N
MOTA	1074	CA	SER	Α	262	55.729	53.610	22.003	1.00	33.31			C
MOTA	1075 -	С	SER	Α	262	56.640	54.837	22.141	1.00	32.60			C
MOTA	1076	0	SER	Α	262	57.725	54.751	22.711	1.00	32.55			0
MOTA	1077	CB	SER	Α	262	54.755	53.566	23.185	1.00	34.17		•	C
MOTA	1078	OG	SER	Α	262	54.108	54.811	23.367	1.00	33.9i			0
ATOM	1079	N	SER	Α	263	56.185	55.986	21.638	1.00	31.57			N
MOTA	1080	CA	SER	Α	263	56.976	57.216	21.715	1.00	31.90			С
MOTA	1081	С	SER	Α	263	56.966	57.806	23.119	1.00	31.13			С
MOTA	1082	0	SER	A	263	57.846	58.585	23.483	1.00	32.42			0
MOTA	1083	СВ			263	56.471	58.265	20.709	1.00	32.36			C
MOTA	1084	OG			263	55.175	58.741	21.027		34.74			0
MOTA	1085	N			264	55.963	57.441	23.905		29.11	•		N
ATOM	1086	CA	ASP			55.864	57.918	25.279		27.37			C
ATOM	1087	C	ASP			55.321	56.786	26.142		26.83			C
ATOM	1088	0.	ASP			54.107	56.594	26.249		26.56			0
ATOM	1089	CB	ASP			54.960	59.156	25.351		26.62			C
ATOM	1090	CG	ASP			54.591	59.538	26.778		25.32			C
MOTA	1091		ASP			55.309	59.148	27.725		23.52			0
MOTA	1092		ASP			53.578	60.243	26.949		25.29			0
ATOM	1093	N			265	56.239	56.036	26.744		25.91			N
ATOM	1093	CA			265	55.868	54.908	27.581		26.10			C
MOTA	1094	CA			265	55.421	55.273	28.981		26.10			C
111 011	1000	_	711	~	200	22.441	22.213	40.201	1.00	40.00			_

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ATOM	1096	0	GLY	A	265	55.005	54.404	29.750	1.00 26.18		0
MOTA	1097	N	PHE	Α	266	55.514	56.551	29.328	1.00 26.34		N
MOTA	1098	CA	PHE	A	266	55.082	56.982	30.650	1.00 26.68		С
MOTA	1099	С	PHE	Α	266	53.564	57.071	30.531	1.00 27.63		С
MOTA	1100	0	PHE-	Α	266	52.988	58.150	30.606	1.00 26.70		0
ATOM	1101	CB	PHE	Α	266	55.677	58.352	30.984	1.00 25.83		C
MOTA	1102	CG	PHE	A	266	55.781	58.634	32.462	1.00 26.28	,	С
ATOM	1103	CD1	PHE	Α	266	55.018	57.915	33.386	1.00 25.02	•	C
MOTA	1104	CD2	PHE	Α	266	56.618	59.647	32.927	1.00 25.66		С
MOTA	1105	CE1	PHE	Α	266	55.083	58.201	34.745	1.00 23.88	-	C
MOTA	1106	CE2	PHE	Α	266	56.694	59.946	34.290	1.00 24.67		C
MOTA	1107	CZ	PHE	А	266	55.923	59.221	35.202	1.00 26.34		С
MOTA	1108	N	SER	Α	267	52.924	55.917	30.338	1.00 29.46		N
ATOM	1109	CA	SER	А	267	51.477	55.855	30.154	1.00 30.33		С
MOTA	1110	C	SER			50.777	54.748	30.930	1.00 31.43		С
ATOM	1111	0	SER			51.302	53.642	31.087	1.00 29.64		0
ATOM	1112	CB	SER			51.160	55.677	28.670	1.00 30.83		С
MOTA	1113	OG	SER			49.775	55.456	28.462	1.00 33.50		0
ATOM	1114	N	GLU			49.572	55.053	31.394	1.00 32.18		N
ATOM	1115	CA	GLU	Α	268	48.783	54.087	32.135	1.00 33.83		С
ATOM	1116	C	GLU			48.483	52.896	31.227	1.00 33.76		С
MOTA	1117	0	GLU			48.289	51.778	31.699	1.00 34.08		0
ATOM	1118	СВ	GLU			47.481	54.729	32.621	1.00 35.26		C
ATOM	1119	CG			268		53.851	33.573	1.00 39.14		С
ATOM	1120	CD	GLU			45.494	54.561	34.188	1.00 41.79		С
ATOM	1121	OE1	GLU			44.761	53.901	34.961	1.00 43.08		0
ATOM	1122	OE2	GLU			45.286	55.767	33.908	1.00 41.44		0
ATOM	1123	N			269	48.458	53.133	29.920	1.00 33.42		N
ATOM	1124	CA			269	48.190	52.058	28.972	1.00 34.58		C
ATOM	1125	C			269	49.255	50.963	29.027	1.00 34.05		C
ATOM	1126	0			269	48.942	49.784	28.846	1.00 33.83		0
ATOM	1127	СВ			269	48.087	52.602	27.543	1.00 36.69		С
ATOM	1128	CG			269	46.919	53.508	27.340	1.00 40.80		С
ATOM	1129	CD1			269	46.944	54.869	27.236	1.00 41.67		C
ATOM	1130	CD2			269	45.540	53.126	27.268	1.00 42.61		С
ATOM	1131		TRP			45.667	55.359	27.106	1.00 43.36		N
ATOM	1132	CE2			269	44.785	54.311	27.123	1.00 43.31		C
ATOM	1133	CE3	TRP			44.868	51.896	27.315	1.00 43.67		С
ATOM	1134.		TRP	A	269	43.390	54.305	27.024	1.00 44.76		С
ATOM	1135		TRP			43.480	51.888	27.216	1.00 44.62		C
ATOM	1136		TRP			42.757		27072	1.00 45.35		С
ATOM	1137	N			270	50.510	51.344	29.257	1.00 32.55		N
MOTA	1138	CA			270	51.582	50.354	29.343	1.00 32.29		С
MOTA	1139	С			270	51.421	49.566	30.641	1.00 31.72		С
ATOM	1140	0			270	51.685	48.368	30.686	1.00 31.18		0
ATOM	1141	CB			270	52.961	51.025	29.314	1.00 31.01		С
MOTA	1142	CG			270	53.207	51.882	28.083	1.00 30.60		C
MOTA	1143	CD			270	54.489	51.525	27.357	1.00 30.06		С
ATOM	1144		GLN			55.390	50.904	27.923	1.00 29.84		0
MOTA	1145		GLN			54.584		26.100	1.00 28.50		N
MOTA	1146	N			271	50.991	50.246	31.698	1.00 32.14		N
ATOM	1147	CA			271	50.782	49.575	32.971	1.00 33.59		. C.
ATOM	1148	C			271	49.694	48.514	32.793	1.00 33.87		С
ATOM	1149	Ō			271	49.838	47.378	33.246	1.00 33.86		0
ATOM	1150	CB			271	50.355	50.568	34.051	1.00 33.76		C
ATOM	1151	CG			271	50.063	49.894	35.384	1.00 35.01		C
ATOM	1152	CD			271	49.834	50.893	36.498	1.00 36.09		C

MOTA	1153	CE	LYS	Α	271	49.709	50.170	37.835	1.00 38.50	C
MOTA	1154	NZ	LYS	А	271	49.561	51.103	38.991	1.00 41.38	N
MOTA	1155	N	ILE	Α	272	48.612	48.895	32.121	1.00 33.39	N
MOTA	1156	CA	ILE	Α	272	47.501	47.987	31.873	1.00 34.07	C
MOTA	1157	C	ILE	Α	272	47.957	46.798	31.034	1.00 33.99	C
ATOM	1158	0	ILE	А	272	47.635	45.653	31.345	1.00 34.22	0
ATOM	1159	CB	ILE	A	272	46.341	48.713	31.145	1.00 33.73	C
MOTA	1160	CG1	ILE	Α	272	45.735	49.768	32.074	1.00 34.18	C
MOTA	1161	CG2	ILE	Α	272	45.281	47.710	30.707	1.00 33.44	C
MOTA	1162		ILE			44.704	50.668	31.413	1.00 34.51	C
MOTA	1163.	N	THR			48.715	47.072	29.977	1.00 33.02	N
MOTA	1164	CA	THR			49.205	46.013	29.104	1.00 33.58	C
MOTA	1165	C	THR			50.099	45.011	29.835	1.00 34.00	C
MOTA	1166	Ō	THR			49.921	43.800	29.697	1.00 33.77	0
MOTA	1167	СВ	THR			49.986	46.595	27.911	1.00 33.70	C
MOTA	1168		THR			49.114	47.426	27.135	1.00 35.34	0
MOTA	1169	CG2				50.521	45.480	27.025	1.00 32.30	c
MOTA	1170	N			274	51.065	45.512	30.599	1.00 32.30	N
ATOM	1171	CA			274	51.969	44.640	31.340	1.00 33.72	C
MOTA	1171	CA			274	51.176	43.843	32.375	1.00 33.04	c
					274					0
MOTA	1173	0				51.414	42.650	32.571	1.00 33.85	
ATOM	1174	CB			274	53.060	45.451	32.071	1.00 33.60	C
ATOM	1175	CG1			274	53.927	46.194	31.051	1.00 33.18	C
ATOM	1176		ILE			53.906	44.521	32.950	1.00 33.23	, C
ATOM	1177		ILE			54.987	47.089	31.674	1.00 33.18	C
ATOM	1178	N			275	50.231	44.513	33.030	1.00 34.87	N
ATOM	1179	CA			275	49.412	43.860	34.036	1.00 36.02	C
ATOM	1180	C			275	48.617	42.686	33.492	1.00 36.38	С
MOTA	1181	0			275	48.494	41.655	34.147	1.00 37.56	0
MOTA	1182	N			276	48.075	42.846	32.292	1.00 36.26	N
MOTA	1183	CA			276	47.292	41.796	31.656	1.00 36.36	C
MOTA	1184	C	TRP	Α	276	48.193	40.601	31.366	1.00 37.31	С
MOTA	1185	0	TRP	A	276	47.788	39.448	31.531	1.00 37.11	0
ATOM	1186	CB	TRP	Α	276	46.701	42.307	30.344	1.00 35.76	C
MOTA	1187	CG	TRP	A	276	45.824	41.316	29.656	1.00 36.30	С
MOTA	1188	CD1	TRP	Α	276	44.483	41.132	29.850	1.00 35.72	С
MOTA	1189	CD2	TRP	Α	276	46.222	40.359	28.665	1.00 35.75	С
MOTA	1190	NE1	TRP	Α	276	44.023	40.121	29.038	1.00 35.15	N
MOTA	1191	CE2	TRP	Α	276	45.067	39.629	28.301	1.00 35.45	C
MOTA	1192	CE3	TRP	Α	276	47.443	40.047	28.050	1.00 35.85	C
MOTA	1193	CZ2	TRP	Α	276	45.094	38.607	27.347	1.00 35.33	C
MOTA	1194	CZ3	TRP	Α	276	47.471	39.027	27.098	1.00 36.37	C
ATOM	1195	CH2	TRP			46.300	38.320	26.758	1.00 36.25	C
ATOM	1196	N			277	49.415	40.885	30.926	1.00 36.56	N
ATOM	1197	CA			277	50.370	39.834	30.607	1.00 36.06	С
ATOM	1198	С			277	50.757	39.048	31.857	1.00 37.15	C
ATOM	1199	0			277	50.865	37.824	31.821	1.00 36.69	ō
ATOM	1200	CB			277	51.636	40.424	29.942	1.00 34.92	C
ATOM	1201		ILE			51.282	40.963	28.550	1.00 34.03	C
MOTA	1202		ILE			52.724	39.363	29.837	1.00 34.05	C
ATOM	1202		ILE			52.412	41.698	27.863	1.00 34.10	C
ATOM	1203	И			277	50.955	39.756	32.962	1.00 32.67	N
ATOM	1204	CA			278		39.736	34.220	1.00 38.15	C
						51.328				
MOTA	1206	C			278	50.198	38.278	34.802	1.00 42.31	. C
MOTA	1207	O CB			278	50.445	37.273	35.468	1.00 42.76	. 0
MOTA	1208	CB			278	51.743	40.189	35.234	1.00 39.40	C
MOTA	1209	CG	AKG	А	278	53.054	40.864	34.911	1.00 38.26	· C

ATOM	1210	CD	ARG	А	278	54.240	39.956	35.206	1.00	37.49	C
MOTA	1211	NE	ARG	Α	278	55.493	40.590	34.802		35.79	N
ATOM	1212	CZ	ARG			56.192	40.250	33.725		34.09	C
MOTA	1213		ARG			55.774	39.267	32.938		33.23	N
MOTA	1214	NH2	ARG			57.298	40.913	33.420		33.05	N
ATOM	1215	N			279	48.962	38.692	34.543		44.10	N
MOTA	1216	CA			279	47.785	37.989	35.039		46.28	C
ATOM	1217	C			279	47.513	36.691	34.282		45.72	C
ATOM	1218	0			279	46.944	35.752	34.832		46.12	0
MOTA	1219	CB			279	46.561	38.903	34.944		48.80	C
ATOM	1220	CG			279	45.260	38.276	35.411		54.66	C
MOTA	1221	CD	GLU			44.101	39.259	35.381		58.25	С
MOTA	1222		GLU			43.781	39.778	34.285		60.30	0
ATOM	1223		GLU			43.511	39.515	36.455		59.99	0
ATOM	1224	N			280	47.927	36.638	33.022		44.85	N
ATOM	1225	CA			280	47.704	35.454	32.207		44.61	C
ATOM	1226	C	LYS			48.924	34.556	32.057		43.52	C
ATOM	1227	0	LYS			48.787	33.361	31.808		44.19	0
ATOM	1228	CB			280	47.212	35.867	30.817		46.41	C
MOTA	1229	CG	LYS			47.082	34.709	29.834		48.70	C
ATOM	1230	CD .	LYS			46.383	35.138	28.550		50.95	C
ATOM	1231	CE			280	46.292	33.987	27.556		51.64	C
ATOM	1232	NZ			280	45.625	32.794	28.148		53.00	N
ATOM	1233	N			281	50.115	35.122	32.217		41.82	N
	1234	CA			281	51.338	34.353	32.050		39.15	С
MOTA	1235	C			281	52.317	34.435	33.216		38.62	С
ATOM	1236	0			281	53.355	33.773	33.198		37.75	0
MOTA	1237	CB			281	52.059	34.816	30.787		38.77	С
ATOM	1238	CG			281	51.280	34.655	29.503	1.00	37.82	C
MOTA	1239	CD1			281	51.167	33.409	28.882		37.09	C
MOTA	1240	CD2				50.693	35.757	28.882		36.24	С
MOTA	1241		TYR			50.498	33.267	27.670		36.51	С
MOTA	1242		TYR			50.019	35.625	27.674		37.22	C
ATOM	1243	CZ			281	49.928	34.378	27.071		37.04	С
MOTA	1244	OH			281	49.284	34.247	25.863		38.46	0
ATOM	1245	N ·	GLY			52.002	35.236	34.225		38.46	N
MOTA	1246	CA			282	52.926	35.370	35.337	1.00	39.34	С
MOTA	1247	C			282	54.249	35.931	34.829		40.34	С
MOTA	1248	0			282	54.262	36.760	33.919		38.99	0
MOTA	1249	N			283	55.360	35.479	35.402		42.07	N
ATOM	1250		ASP			56.682	35.945	34.990		44.04	C
MOTA	1251	C	ASP			57.306	35.069	33.905		44.08	C
ATOM	1252	O ·	ASP			58.510	35.130	33.674		44.67	0
ATOM	1253	CB	ASP			57.629	35.994	36.193		45.90	С
MOTA	1254	CG	ASP			57.267	37.087	37.180		49.98	С
ATOM	1255		ASP			57.233	38.274	36.777		51.56	0
MOTA	1256	OD2	ASP			57.023	36.760	38.363		52.17	0
ATOM	1257	N			284	56.493	34.260	33.236		44.69	N
ATOM	1258	CA			284	57.000	33.373	32.191		45.15	C
MOTA	1259	С			284	57.172	34.086	30.854		43.68	С
ATOM	1260	0			284	57.955	33.664	30.001		44.14	0
ATOM	1261	CB			284	56.064	32.171	32.024		48.63	С
MOTA	1262	CG			284	56.003	31.260	33.249		53.02	С
ATOM	1263	CD			284	57.377	30.674	33.572		56.22	С
ATOM	1264	CE			284	57.326	29.736	34.772		58.58	С
ATOM	1265	NZ			284	58.679	29.181	35.089		60.63	N
MOTA	1266	N	VAL	A	285	56.425	35.164	30.669	1.00	40.25	N

MOTA	1267	CA	VAL	A	285	56.514	35.937	29.446	1.00 37.27		С
ATOM	1268	С	VAL	A	285	57.225	37.243	29.773	1.00 35.62		С
ATOM	1269	0	VAL	A	285	56.792	37.997	30.641	1.00 35.11		0
MOTA	1270	CB	VAL	А	285	55.114	36.213	28.874	1.00 37.07		С
ATOM	1271	CG1	VAL	Α	285	55.205	37.182	27.706	1.00 35.98		С
ATOM	1272	CG2	VAL	A	285	54.489	34.897	28.418	1.00 37.05		C
ATOM	1273	N	LYS			58.331	37.494	29.084	1.00 34.12		N
MOTA	1274	CA	LYS			59.117	38.699	29.311	1.00 31.70		С
ATOM	1275	С	LYS			58.643	39.823	28.404	1.00 30.65		C
ATOM	1276	0	LYS			58.443	39.625	27.206	1.00 29.79		0
ATOM	1277	CB	LYS			60.599	38.411	29.059	1.00 30.46		С
ATOM	1278	CG	LYS			61.135	37.224	29.847	1.00 30.11	•	С
ATOM	1279	CD	LYS			60.902	37.387	31.344	1.00 29.65		С
ATOM	1280	CE	LYS			61.427	36.183	32.118	1.00 29.40		С
ATOM	1281	NZ	LYS			61.201	36.319	33.591	1.00 30.72		N
MOTA	1282	N	VAL			58.469	41.005	28.983	1.00 28.78		N
ATOM	1283	CA	VAL			58.004	42.154	28.224	1.00 27.93		C
ATOM	1284	C	VAL			58.722	43.442	28.617	1.00 27.40		Ċ
MOTA	1285	0	VAL			58.733	43.838	29.784	1.00 26.80		ō
ATOM	1286	CB	VAL			56.463	42.338	28.400	1.00 27.55		C
ATOM	1287				287	56.102	42.398	29.876	1.00 27.53		C
MOTA	1288		VAL			56.002	43.603	27.704	1.00 28.04		C
ATOM	1289	N			288	59.340	44.081	27.630	1.00 28.27		N
MOTA	1290	CA			288	60.031	45.336	27.873	1.00 27.27		C
MOTA	1291	C			288	59.038	46.459	27.644	1.00 27.27		C
ATOM	1291	0	GLY			58.042	46.263	26.944	1.00 27.80		0
ATOM	1292	N			289	59.293	47.627	28.230	1.00 23.10		И
											C
ATOM	1294	CA	ALA			58.396	48.771	28.085	1.00 28.35		C
ATOM	1295	C			289	59.171	50.063	27.815	1.00 29.42		
MOTA	1296	0			289	60.386	50.120	28.021	1.00 29.84		0
MOTA	1297	CB	ALA			57.543	48.923	29.346	1.00 28.05		C
ATOM	1298	N			290	58.461	51.096	27.364	1.00 28.77		N
MOTA	1299	CA			290	59.096	52.371	27.063	1.00 28.22		C
ATOM	1300	C			290	58.395	53.070	25.905	1.00 28.36		C
ATOM	1301	0			290 .	57.369	52.588	25.433	1.00 27.76		0
MOTA	1302	N			291.	58.942	54.184	25.418	1.00 26.86	•	N
MOTA	1303	CA			291	60.186	54.766	25.919	1.00 25.60		C
ATOM	1304	C			291	59.985	55.857	26.969	1.00 25.05		C
ATOM	1305	0			291	58.963	56.536	26.987	1.00 25.04		0
ATOM.	1306	CB			291	60.973	55.357	24.748	1.00 24.30		C
ATOM	1307	CG	ASN			61.485	54.298	23.793	1.00 24.09		C
MOTA	1308		ASN			60.978	53.180	23.761	1.00 25.26		0
ATOM	1309		ASN			62.492	54.651	23.001	1.00 20.96		И
ATOM	1310	N			292	60.965	56.010	27.852	1.00 23.64		N
ATOM	1311	CA			292	60.923	57.054	28.867	1.00 23.62		C
ATOM	1312	C			292	62.290	57.733	28.846	1.00 24.18		С
ATOM	1313	0			292	63.219	57.230	28.200	1.00 24.40		0
ATOM	1314	СВ			292	60.583	56.498	30.289	1.00 24.12		C
ATOM	1315		ILE			61.395	55.238	30.599	1.00 23.86		C
ATOM	1316		ILE			59.093	56.210	30.383	1.00 24.23		C
ATOM	1317		ILE			62.865	55.491	30.874	1.00 24.33		С
MOTA	1318	N			293	62.420	58.870	29.528	1.00 22.80		N
ATOM	1319	CA			293	63.686	59.597	29.526	1.00 22.92		C
ATOM	1320	С			293	64.146	60.119	30.876	1.00 23.26		C
ATOM	1321	0			293	65.142	60.840	30.951	1.00 23.53		0
ATOM	1322	CB			293	63.635	60.805	28.561	1.00 22.53		C
ATOM	1323	CG1	VAL	A	293	63.492	60.330	27.122	1.00 21.53		С

MOTA	1324	CG2	VAL	A	293	62.474	61.717	28.943	1.00 21.31		С
MOTA	1325	N	ASP	А	294	63.430	59.779	31.942	1.00 23.20		N
MOTA	1326	CA			294	63.824	60.241	33.269	1.00 23.65		C
MOTA	1327	C	ASP	A	294	63.528	59.203	34.352	1.00 24.09,		С
ATOM (	1328	0	ASP	Α	294	62.885	58.188	34.096	1.00 24.41		0
MOTA	1329	CB	ASP	Α	294	63.122	61.570	33.597	1.00 23.02		С
MOTA	1330	CG	ASP	Α	294	61.620	61.418	33.778	1.00 24.10		C
MOTA	1331	OD1	ASP	Α	294	61.064	60.375	33.376	1.00 26.12		.0
ATOM	1332	OD2	ASP	Α	294	60.990	62.354	34.312	1.00 25.00		0
MOTA	1333	N	GLY	Α	295	64.006	59.467	35.561	1.00 25.18		N
MOTA	1334	CA	GLY	A	295	63.793	58.553	36.669	1.00 25.72		Ċ
ATOM	1335	C	GLY	Α	295	62.339	58.246	36.987	1.00 26.61		С
MOTA	1336	0	GLY	Α	295	62.016	57.105	37.326	1.00 25.47		0
MOTA	1337	N	GLU	Α	296	61.463	59.249	36.894	1.00 27.36		N
MOTA	1338	CA	GLU	Α	296	60.042	59.049	37.184	1.00 28.17		С
ATOM	1339	С	GLU	Α	296	59.417	58.064	36.214	1.00 26.97		С
MOTA	1340	0	GLU	Α	296	58.684	57.166	36.620	1.00 26.88		0
ATOM	1341	CB	GLU	Α	296	59.261	60.367	37.103	1.00 31.11		С
ATOM	1342	CG	GLU	Α	296	59.579	61.376	38.182	1.00 37.71		С
ATOM	1343	CD	GLU	A	296	58.622	62.567	38.160	1.00 43.64		C
MOTA	1344	OE1	GLU	А	296	58.943	63.589	38.808	1.00 45.94		0
MOTA	1345	OE2	GLU	Α	296	57.550	62.482	37.503	1.00 44.55		0
ATOM	1346	N	GLY	Α	297	59.695	58.251	34.928	1.00 26.28		N
MOTA	1347	ÇA	GLY	Α	297	59.151	57.363	33.917	1.00 26.08		С
MOTA	1348	C			297	59.661	55.944	34.094	1.00 25.81		С
ATOM	1349	0	GLY	Α	297	58.910	54.984	33.932	1.00 26.85		0
ATOM	1350	N			298	60.945	55.813	34.415	1.00 25.29		N
MOTA	1351	CA			298	61.554	54.506	34.639	1.00 25.86		С
MOTA	1352	,C			298	60.856	53.815	35.805	1.00 26.44		C
MOTA	1353	0			298	60.461	52.656	35.712	1.00 26.85		0
MOTA	1354	CB	PHE	Α	298	63.040 ·	54.655	34.988	1.00 25.61		C
ATOM	1355	CG	PHE	A	298	63.640	53.410	35.585	1.00 25.67		C
ATOM	1356	CD1	PHE	Α	298	64.139	52.398	34.771	1.00 24.15	•	С
MOTA	1357		PHE			63.627	53.214	36.964	1.00 24.54		C
ATOM	1358	CE1	PHE	Α	298	64.611	51.202	35.325	1.00 24.57		C
MOTA	1359	CE2	PHE	A	298	64.093	52.025	37.524	1.00 24.83	•	C
MOTA	1360	CZ	PHE	À	298	64.584	51.017	36.701	1.00 23.36		С
MOTA	1361	N	ARG	A	299	60.733	54.553	36.905	1.00 27.12		N
MOTA	1362	CA	ARG			60.110	54.089	38.143	1.00 29.07		С
MOTA	1363	C	ARG	A	299	58.680	53.603	37.910	1.00 29.11		С
MOTA	1364	0	ARG	Α	299	58.275	52.554	38.420	1.00 28.93		0
MOTA	1365	CB	ARG	A	.299	60.136	55.235	39.162	1.00 30.82		С
MOTA	1366	CG	ARG	Α	299	59.233	55.085	40.370	1.00 35.20		C
MOTA	1367	CD	ARG	A	299	59.914	54.374	41.518	1.00 38.25		С
MOTA	1368	NE	ARG	Α	299	61.166	55.010	41.934	1.00 39.66		N
MOTA	1369	CZ	ARG	A	299	61.900	54.581	42.959	1.00 40.55		С
MOTA	1370	NH1	ARG	А	299	61.497	53.533	43.662	1.00 39.93		N
MOTA	1371	NH2	ARG	Α	299	63.045	55.173	43.270	1.00 40.75		N
MOTA	1372	N	TYR	Α	300	57.912	54.363	37.139	1.00 28.00		N
ATOM	1373	CA	TYR			56.542	53.973	36.853	1.00 27.38		C
MOTA	1374	С	TYR			56.486	52.639	36.113	1.00 27.60		` C
MOTA	1375	0	TYR			55.658	51.793	36.424	1.00 27.82		0
MOTA	1376	CB	TYR			55.841	55.033	36.006	1.00 25.95		С
MOTA	1377	CG	TYR			54.385	54.714	35.739	1.00 25.23		C
MOTA	1378	CD1	TYR	Α	300	53.410	54.933	36.716	1.00 24.39		C
MOTA	1379	CD2	TYR	A	300	53.984	54.183	34.516	1.00 24.30		С
MOTA	1380	CE1	TYR	Α	300	52.069	54.631	36.477	1.00 23.68		С

ATOM	1381	CE2	TYR Z	A	300	52.650	53.875	34.268	1.00			C
ATOM	1382	CZ	TYR .	A	300	51.698	54.104	35.252	1.00			C
ATOM	1383	OH	TYR .	A	300	50.379	53.810	34.995	1.00			0
ATOM	1384	N	LEU .	Α	301	57.355	52.454	35.124	1.00			N
MOTA	1385	CA	LEU .	Α	301	57.339	51.210	34.369	1.00			С
MOTA	1386	C	LEU .	Α	301	57.922	50.044	35.168	1.00			С
MOTA	1387	0	LEU .	A	301	57.539	48.896	34.968	1.00			0
MOTA	1388	CB	LEU .	Α	301	58.078	51.386	33.036	1.00	25.33		C
ATOM	1389	CG	LEU .	Α	301	57.369	52.305	32.024	1.00	25.53		C
ATOM `	1390	CD1	LEU .	Α	301	58.189	52.409	30.741	1.00	20.77		С
MOTA	1391	CD2	LEU	Α	301	55.979	51.756	31.714	1.00	23.64		С
ATOM	1392	N	ALA.	Α	302	58.837	50.340	36.081	1.00	28.68		N
MOTA	1393	CA	ALA	Α	302	59.437	49.301	36.911	1.00	29.55		C
MOTA	1394	С	ALA	Α	302	58.365	48.740	37.852	1.00	29.73		С
ATOM	1395	0	ALA			58.159	47.528	37.925	1.00	29.99		0
MOTA	1396	CB	ALA			60.607	49.877	37.714	1.00	27.04		C
ATOM		N	ASP			57.679	49.624	38.565	1.00	30.56		N
ATOM	1398	CA	ASP			56.625	49.193	39.474	1.00	31.48		C
ATOM	1399	C			303	55.527	48.474	38.704	1.00	32.09		C
ATOM	1400	Ö	ASP			54.836	47.620	39.256	.1.00	33.91		0
ATOM	1401	СВ	ASP			56.013	50.381	40.218	1.00	31.91		. C
ATOM	1402	-CG	ASP			56.947	50.968	41.254	1.00	33.42		C
ATOM	1402		ASP			57.869	50.253	41.701		34.40		0
	1403		ASP			56.743	52.139	41.639		34.93		0
ATOM ATOM		N	ALA			55.358	48.828	37.434		31.62		N
	1405		ALA			54.336	48.198	36.605		30.73		C
ATOM	1406	CA				54.723	46.759	36.239		30.76		C
MOTA,	1407	C	ALA			53.873	45.969	35.823		30.18		Ō
ATOM	1408	0	ALA				49.020	35.346		30.45		C
ATOM	1409	CB	ALA			54.103	46.425	36.379		29.89		N
ATOM	1410	N	GLY			56.007	45.069	36.086		28.06		C
MOTA	1411	CA	GLY			56.452	44.817	34.850		28.84		C
MOTA	1412	C	GLY			57.299	43.661	34.535		28.23		0
MOTA	1413	0			305	57.596	45.873	34.144		28.22		N
MOTA	1414	N			306	57.695	45.719	32.937		27.85		C
ATOM	1415	CA			306	58.510		33.206		27.06		C
MOTA	1416	C			306	59.772	44.889	34.270		26.25		Ô
MOTA	1417	0			306	60.378	45.010			28.08		C
ATOM	1418	CB			306	58.896	47.094	32.399		27.17	٠.	N
ATOM	1419	N	•		307	60.157	44.049	32.244		27.17	•	C
MOTA	1420	CA			307	61.350	43.201	32.374		27.07		C
MOTA	1421	C			307	62.618	43.950	31.946		27.56		0
MOTA	1422	0			307	63.737	43.546				*	C
MOTA	1423	CB			307	61.178	41.918	31.553		26.85		C
ATOM	1424	CG			307	60.190	40.954	32.187		29.12		0
MOTA	1425		ASP			60.488	40.450	33.290		29.15		0
MOTA	1426		ASP			59.116	40.709	31.592		29.54	•	
MOTA	1427	N			. 308	62.424	45.021	31.189		26.81		N
MOTA	1428				308	63.507	45.896	30.771		26.08		C
MOTA	1429	C			. 308	62.823	47.180	30.314		26.24		C
MOTA	1430	0			308	61.677	47.158	29.871		25.83		0
MOTA	1431	CB			308	64.416	45.245	29.703		25.02		C
ATOM	1432	CG			308	63.879	45.264	28.291		24.83		C
MOTA	1433		PHE			63.847	46.447	27.552		24.91		C
MOTA	1434	CD2	PHE	A	308	63.492	44.076	27.671		24.33		C
ATOM	1435		PHE			63.443		26.210		24.84		C
ATOM	1436	CE2	PHE	A	308	63.085				25.69		C
ATOM	1437	CZ	PHE	A	308	63.062	45.255	25.597	1.00	25.81		С
									•			

MOTA	1438	N	ILE	A	309	63.503	48.305	30.484	1.00	25.90		N
ATOM	1439	CA	ILE			62.928	49.591	30.130	1.00	25.03		C
ATOM	1440	С	ILE			63.754	50.294	29.053		24.57	•	C
MOTA	1441	0	ILE			64.976	50.407	29.160	1.00	24.32		0
MOTA	1442	CB	ILE			62.784	50.445	31.414		25.42		C
ATOM	1443	CG1	ILE			61.756	49.763	32.331		22.98		С
ATOM	1444	CG2	ILE			62.390	51.891	31.072		24.21		C
ATOM	1445		ILE			61.674	50.320	33.740		22.68		C
ATOM	1446	N	LYS			63.068	50.750	28.009		24.43		N
ATOM	1447	CA	LYS			63.713	51.396	26.877		24.50		C
ATOM	1448	C	LYS			63.785	52.921	27.042		24.35		C
ATOM	1449	0			310	62.786	53.583	27.334		23.81		0
	1450	CB	LYS			62.780	51.000	25.598		24.83		C
MOTA							51.000			24.74		C
ATOM	1451	CG	LYS			63.793		24.336		24.74		C
ATOM	1452	CD	LYS			63.473	49.906	23.401				C
ATOM	1453	CE	LYS			62.069	49.994	22.836		24.22		
ATOM	1454	NZ	LYS			61.904	51.272	22.092		23.28		N
MOTA	1455	N			311	64.986	53.459	26.851		23.88		N
ATOM	1456		ILE			65.252	54.890	27.009		23.05		C
ATOM	1457	С	ILE			65.399	55.641	25.693		23.48		С
MOTA	1458	0			311	66.113	55.194	24.792		22.99		0
MOTA	1459	CB			311	66.562	55.118	27.804		21.85		С
ATOM	1460	CG1	ILE			66.503	54.367	29.137		19.66	•	C
MOTA	1461	CG2	ILE	A	311	66.782	56.619	28.037	1.00	19.08		С
MOTA	1462	CD1	ILE	Α	311	67.858	54.239	29.821		19.70		С
ATOM	1463	N	GLY	А	312	64.730	56.785	25.582	1.00	23.63		N
MOTA	1464	CA	GLY	Α	312	64.871	57.569	24.374	1.00	24.66		C
MOTA	1465	C	GLY	А	312	63.644	58.103	23.669	1.00	26.40		C
ATOM	1466	0	GLY	Α	312	62.771	57.350	23.240	1.00	25.18		0
MOTA	1467	N	ILE	Α	313	63.595	59.426	23.553	1.00	28.70		N
MOTA	1468	CA	ILE	Α	313	62.527	60.128	22.854	1.00	31.54	•	C
ATOM	1469	С	ILE	A	313	63.184	61.309	22.152	1.00	35.25		C
MOTA	1470	O			313	63.698	62.216	22.811	1.00	33.97		0
MOTA	1471	CB			313	61.450	60.678	23.812	1.00	30.50		C
ATOM	1472	CG1			313	60.739	59.528	24.529	1.00	29.70		C
ATOM	1473		ILE			60.438	61.498	23.021	1.00	30.02		Ċ
MOTA	1474		ILE			59.794	59.984	25.624	1.00	27.55		С
ATOM	1475	N			314	63.190	61.283	20.823		40.22		N
ATOM	1476	CA			314	63.780	62.372	20.065		47.64		C
MOTA	1477	C			314	65.152	62.121	19.458		53.44		C
MOTA	1478	0			314	65.474		18.392		54.62		0
ATOM	1479	N			315	65.965	61.306	20.125	1.00	57.31		N
ATOM .	1480	CA			315		61.024	19.632		62.24		C
ATOM	1481	C			315	67.422	60.395	18.251		65.54		C
MOTA	1482	0			315	68.347	60.724	17.509		66.23		0
ATOM	1483	N			316	66.499	59.497	17.906		68.35		N
MOTA	1484	CA			316	66.534	58.826	16.611		71.80		C
MOTA	1485	C			316	66.996	59.648	15.415		74.31		C
ATOM					316	66.889	60.875	15.413		74.26		0
	1486	O N					58.968	14.388		76.73		N
ATOM	1487	N C7			317	67.505						
ATOM	1488	CA			317	67.989	59.635	13.178		79.34		C
ATOM	1489	C			317	66.831	60.196	12.357		81.34		C
ATOM	1490	0			317	66.887	61.330	11.879		81.51		0
MOTA	1491	CB			317	68.799	58.663	12.314		79.01		C
ATOM	1492	OG			317	67.969	57.683	11.719		78.20		0
ATOM	1493	N			318	65.789	59.387	12.189		83.77		N
MOTA	1494	CA	ILE	A	318	64.602	59.797	11.444	1.00	86.14		С

ATOM	1495	C	ILE	Α	318	63.663	60.558	12.371	1.00	87.68			С
ATOM	1496	0	ILE	Α	318	62.441	60.481	12.236	1.00	87.87			0
ATOM	1497	CB	ILE	Α	318	63.845	58.575	10.866	1.00	85.84			C
ATOM	1498	CG1	ILE			64.062	57.346	11.756		85.74			С
ATOM	1499		ILE			64.323	58.291	9.448		86.18			С
ATOM	1500		ILE			63.713	57.544	13.210		84.97			C
MOTA	1501	N	CYS			64.250	61.293	13.312		89.77			N
													C
ATOM	1502	CA	CYS			63.484	62.064	14.282		91.80			
MOTA	1503	C	CYS			63.660	63.571	14.135		92.66			C
MOTA	1504	0	CYS			64.776	64.090	14.207		92.78			0
ATOM	1505	CB	CYS			63.878	61.660	15.703		92.28			С
ATOM	1506	SG	CYS			63.009	62.593	16.985		94.56			s
MOTA	1507	N	ILE	Α	320	62.545	64.268	13.937	1.00	93.64			N
MOTA	1508	CA	ILE	Α	320	62.552	65.720	13.800	1.00	94.66			C
MOTA	1509	C	ILE	A	320	61.771	66.290	14.988	1.00	94.85			С
MOTA	1510	0	ILE	Α	320	60.809	67.041	14.814	1.00	95.16			0
ATOM	1511.	CB	ILE	Α	320	61.876	66.165	12.473	1.00	95.15			С
ATOM	1512	CG1	ILE			62.418	65.339	11.299	1.00	95.39			С
ATOM	1513	CG2	ILE			62.132	67.649	12.226		94.99			С
ATOM	1514		ILE			63.920	65.452	11.086		95.47			Ċ
ATOM	1515	N	THR			62.200	65.913	16.193		94.85			N
ATOM	1516	CA	THR			61.572	66.338	17.446		94.56			C
										94.12			C
ATOM	1517	C	THR			60.932	67.723	17.389					
ATOM	1518	0	THR			59.744	67.876	17.683		93.67			0
MOTA	1519	CB	THR			62.590	66.322	18.606		94.80			С
MOTA	1520		THR			63.228	65.040	18.664		94.77			0
ATOM	1521	CG2	THR			61.891	66.588	19.931		94.58			C
ATOM	1522	N	ARG	A	322	61.721	68.730	17.022	1.00	93.60			N
MOTA	1523	CA	ARG	Α	322	61.208	70.091	16.926	1.00	92.93			С
MOTA	1524	C	ARG	Α	322	59.929	70.126	16.098	1.00	91.61			С
MOTA	1525	0	ARG	Α	322	58.860	70.457	16.611	1.00	91.89			0
MOTA	1526	CB	ARG	Α	322	62.250	71.025	16.301	1.00	93.99			C
ATOM	1527	CG	ARG	A	322	63.301	71.546	17.274	1.00	95.47			C
ATOM	1528	CD	ARG			64.337	70.495	17.640	1.00	96.98	•		С
MOTA	1529	NE	ARG			65.319	71.030	18.583		98.14			N
MOTA	1530	CZ	ARG			66.530	70.517	18.784		98.80			С
ATOM	1531		ARG			66.925	69.448	18.105		98.87			N
ATOM	1532		ARG			67.348	71.079	19.663		99.15			N
ATOM	1533	N	GLU			60.036	69.778	14.820		89.52			N
•													
MOTA	1534	CA	GLU			58.871	69.778	13.946		87.37			C
MOTA	1535	C			323		68.588	14.247		84.86			C
ATOM	1536	0	GLU			57.628	67.795	13.361		84.93			0
MOTA	1537	CB	GLU			59.311	69.757	12.478		88.77			C
MOTA	1538	CG	GLU			58.163	69.856	11.473		90.52			C
MOTA	1539	CD	GLU			57.281	71.080	11.689		91.42			C
MOTA	1540	OE1	GLU	Α	323	56.303	71.245	10.927	1.00	91.57			0
MOTA	1541	OE2	GLU	Α	323	57.560	71.875	12.615	1.00	91.76			0
MOTA	1542	N	GLN	Α	324	57.553	68.473	15.509	1.00	81.41			N
ATOM	1543	CA	GLN	Α	324	56.676	67.393	15.944	1.00	77.43			С
MOTA	1544	С	GLN			55.848	67.831	17.153	1.00	73.46			С
MOTA	1545	0	GLN			54.919	68.630	17.018		73.89			0
ATOM	1546	CB	GLN			57.503	66.146	16.289		79.24			C
ATOM	1547	CG	GLN			56.677	64.923	16.679		81.03			C
ATOM	1548	CD	GLN			55.595	64.599	15.665		82.58			C
ATOM	1549		GLN			55.867	64.472	14.471		83.19		•	0
ATOM		NE2				54.359							И
	1550						64.463	16.137		83.06			
ATOM	1551	N	LYS	A	323	56.191	67.312	18.329	1.00	67.65			N

ATOM	1552	CA	LYS	A	325	55.476	67.644	19.556	1.00	61.35		С
MOTA	1553	C	LYS	Α	325	56.326	68.484	20.492	1.00	56.32		С
MOTA	1554	0	LYS	A	325	55.807	69.147	21.391	1.00	55.43		0
MOTA	1555	CB	LYS	Α	325	55.056	66.375	20.299	1.00	62.67		С
MOTA	1556	CG	LYS	Α	325	53.889	65.612	19.697	1.00	63.57		С
ATOM	1557	CD	LYS	Α	325	53.512	64.469	20.624	1.00	64.06		С
MOTA	1558	CE	LYS	Α	325	52.278	63.738	20.158	1.00	64.95		С
ATOM	1559	NZ	LYS	Α	325	51.932	62.638	21.100	1.00	65.54		N
ATOM	1560	N	GLY	Α	326	57.636	68.444	20.292	1.00	50.41		N
ATOM	1561	CA	GLY	Α	326	58.515	69.204	21.152	1.00	44.73		С
ATOM	1562	С	GLY	Α	326	58.777	68.502	22.473	1.00	41.12		С
ATOM	1563	0	GLY	Α	326	59.036	69.151	23.484	1.00	38.92		0
ATOM	1564	N	ILE	A	327	58.684	67.174	22.474	1.00	37.83		N
ATOM	1565	CA	ILE	Α	327	58.954	66.403	23.680	1.00	34.93		С
ATOM	1566	C			327	60.248	65.627	23.449	1.00	32.50		C
ATOM	1567	0			327	60.556	65.229	22.329		30.63		0
MOTA	1568	СВ			327	57.807	65.406	24.022		35.16		С
MOTA	1569	CG1			327	57.684	64.340	22.936	1.00	35.16		С
ATOM	1570	CG2	ILE			56.485	66.157	24.169	1.00	36.07		C
ATOM	1571		ILE			56.624	63.273	23.233		37.60		C
MOTA	1572		GLY			61.018	65.429	24.507		30.83		N
ATOM	1573	CA			328	62.257	64.695	24.351		30.46		C
MOTA	1574	C			328	63.331	65.116	25.326		28.07		C
ATOM	1575	0			328 .	63.087	65.907	26.241		26.85		Ō
ATOM	1576	N			329	64.531	64.587	25.121		27.11		N
MOTA	1577	CA			329	65.650	64.897	25.991		25.00		C
ATOM	1578	C			329	66.912	64.341	25.355		24.52		C
ATOM	1579	Õ			329	66.866	63.282	24.728		24.57		Ō
MOTA	1580	CB			329	65.426	64.243	27.356		25.02		C
ATOM	1581	CG			329	66.250	64.828	28.486		23.52		C
ATOM	1582	CD			329	66.101	63.994	29.745		23.12		C
ATOM	1583	NE.			329	66.454	64.757	30.935		23.07		N
ATOM	1584	CZ			329	66.352	64.300	32.177		24.79		C
ATOM	1585		ARG			65.909	63.067	32.402		25.05		N
ATOM	1586		ARG			66.670	65.086	33.198		23.95		N
ATOM	1587	N			330	68.031	65.053	25.502		22.80		N
ATOM	1588	CA			330	69.281	64.560	24.952		21.71		C
ATOM	1589	C			330	69.466	63.134	25.449		22.12		C
ATOM	1590	.0			330	69.269	62.856	26.635		21.20		. 0
ATOM	1591	N			331	69.844	62.230	24.552		22.96		N
ATOM	1592	CA	GLN			70.005	60.824	24.900		23.04	16.1	C
ATOM	1593	C	*		331	70.969	60550	26.054		23.91		Ċ
ATOM	1594	Õ			331	70.689	59.699	26.901		24.69		0
ATOM	1595	СВ			331	70.440	60.023	23.670		23.45		Ċ
ATOM	1596	CG			331	70.322	58.504	23.848		23.57		C
ATOM	1597	CD			331	68.876	58.025	23.890		26.07		C
ATOM	1598		GLN			68.595	56.889	24.278		28.19		Ō
ATOM	1599		GLN			67.954	58.887	23.483		23.86		N
ATOM	1600	N			332	72.098	61.256	26.096		22.41		N
ATOM	1601	CA			332	73.068	61.042	27.169		22.13		C
ATOM	1602	C			332	72.460	61.375	28.529		21.81		C
ATOM	1603	0			332	72.528	60.581	29.472		20.89		0
ATOM	1604	CB			332	74.326	61.886	26.928		21.50		C
ATOM	1605	N			333	71.857	62.553	28.626		20.86		N
ATOM	1606	CA			333	71.239	62.979	29.867		21.05		C
ATOM	1607	C				70.148	61.998	30.276		22.50		C
ATOM	1608	0			333	70.013	61.668	31.456		22.49		ō
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ATOM	1609	CB	THR	A	333	70.622	64.384	29.730	1.00	20.97		С
MOTA	1610	OG1	THR	A	333	71.643	65.308	29.334	1.00	19.27		0
MOTA	1611	CG2	THR	A	333	70.023	64.839	31.069	1.00	20.51		C
MOTA	1612	N	ALA	A	334	69.378	61.529	29.297	1.00	21.69		N
MOTA	1613	CA	ALA	A	334	68.299	60.583	29.568	1.00	22.09		С
MOTA	1614	C	ALA	Α	334	68.835	59.278	30.163	1.00	21.26		C
MOTA	1615	0	ALA	Α	334	68.314	58.780	31.160	1.00	22.26		0
ATOM	1616	CB	ALA	A·	334	67.521	60.290	28.281	1.00	20.13		C
MOTA	1617	N			335	69.866	58.721	29.539		22.35		N
MOTA	1618	CA	VAL			70.458	57.469	30.010		22.27		C
MOTA	1619	C			335	71.061	57.628	31.404		22.75		С
ATOM	1620	0	VAL			70.810	56.814	32.298		24.25		0
MOTA	1621	CB	VAL			71.561	56.965	29.041		22.72		С
ATOM	1622		VAL			72.273	55.739	29.639		23.71	•	С
ATOM '	1623		VAL			70.945	56.602	27.702		21.59		C
MOTA	1624	N			336	71.848	58.680	31.590		22.45		N
MOTA	1625	CA			336	72.489	58.930	32.876		22.52		C
ATOM	1626	C			336	71.465	59.051	34.004		23.41		C
MOTA	1627	0			336	71.662	58.518	35.095		22.49		Ō
ATOM	1628	CB			336	73.349	60.217	32.817		21.60		C
MOTA	1629	CG1				74.548	59.985	31.890		19.73		Ċ
ATOM	1630	CG2	ILE			73.804	60.623	34.220		18.66		C
ATOM	1631	CD1	ILE			75.364	61.233	31.615	1.00	21.73		Ċ
ATOM	1632	N			337	70.364	59.742	33.730		24.43		N
ATOM	1633	CA	ASP			69.319	59.938	34.729		24.42		C
ATOM	1634	C			337	68.550	58.646	35.026		24.54		C
ATOM	1635	Ö			337	68.294	58.317	36.186		23.43		Ö
ATOM	1636	СВ			337	68.364	61.038	34.260	1.00			C
MOTA	1637	CG			337	67.298	61.359	35.285		28.42		C
ATOM	1638		ASP			67.631	61.405	36.483		31.45		0
ATOM	1639		ASP			66.131	61.578	34.897		29.42		Ö
ATOM	1640	N			338	68.187	57.912	33.980		24.02		N
MOTA	1641	CA	VAL			67.457	56.664	34.161		23.68		C
ATOM	1642	C	VAL			68.326	-55.622	34.868		24.05		C
MOTA	1643	Ō	VAL			67.842	54.896	35.735		23.76		Ö
ATOM	1644	CB	VAL			66.956	56.110	32.800	1.00	24.17		C
ATOM	1645		VAL			66.387	54.704	32.973		22.42		C
ATOM	1646		VAL			65.882	57.046	32.228		21.26		Č
ATOM	1647	N	VAL			69.607	55.562	34.505		23.11		N
ATOM	1648	CĄ	VAL			70.533	54.614	35.117		23.44		C
ATOM	1649	C			339	70.680	54.852	36.624		24.25		C
ATOM	1650	0			339	70.759	53.898	37.397		25.77		0
ATOM	1651	CB			339	71.930	54.683	34.444		23.37		Ċ
MOTA	1652		VAL			72.970	53.969	35.290		21.96		Ċ
MOTA	1653		VAL			71.866	54.039	33.067		21.79		C
ATOM	1654	N			340	70.719	56.114	37.043		23.85		Ŋ
ATOM	1655	CA			340	70.844	56.428	38.464		24.36		C
ATOM	1656	C.			340	69.579	55.983	39.200		24.66		c
ATOM	1657	0			340	69.645	55.467	40.315		24.46		0
ATOM	1658	CB	ALA			71.068	57.923	38.661		22.34		C
ATOM	1659	N			341	68.426	56.179	38.571		24.16		N
ATOM	1660	CA			341	67.170	55.784	39.188		25.70		C
ATOM	1661	C			341	67.116	54.261	39.261		25.09		C
ATOM	1662	0			341	66.681	53.701	40.258		24.84		0
ATOM	1663	CB	GLU			65.980	56.309	38.375		26.08		C
ATOM	1664	CG			341	64.630	56.199	39.082		27.72		C
ATOM	1665	CD			341	64.541	57.095	40.311		31.11	•	C
			0			52.512	2					_

MOTA	1666	OE1	GLU	Α	341	65.068	58.227	40.269	1.00 32.05		0
MOTA	1667	OE2	GLU	Α	341	63.929	56.680	41.315	1.00 31.72		0
ATOM	1668	N	ARG	Α	342	67.558	53.601	38.195	1.00 25.02		N
ATOM	1669	CA	ARG	Α	342	67.567	52.141	38.137	1.00 25.81		C
ATOM	1670	C	ARG			68.459	51.563	39.241	1.00 25.77		. C
ATOM	1671	Ō	ARG			68.101	50.572	39.869	1.00 25.65		0
	1672	CB	ARG			68.045	51.676	36.752	1.00 24.80		Ċ
ATOM								36.495	1.00 24.72		C
ATOM	1673	CG	ARG			67.994	50.162				C
MOTA	1674	CD	ARG			69.246	49.441	37.015	1.00 23.36		
ATOM	1675	NE	ARG			70.486	49.936	36.413	1.00 22.99		N
ATOM	1676	CZ	ARG	Α	342	70.856	49.729	35.149	1.00 23.14		C
MOTA	1677	NH1	ARG	Α	342	70.086	49.028	34.325	1.00 23.28		N
MOTA	1678	NH2	ARG	Α	342	72.002	50.227	34.701	1.00 22.15		N
MOTA	1679	N	ASN	A	343	69.609	52.189	39.481	1.00 25.74		N
MOTA	1680	CA	ASN	Α	343	70.524	51.722	40.519	1.00 26.49		С
MOTA	1681	C	ASN	Α	343	69.928	51.972	41.899	1.00 28.14		C
ATOM	1682	0	ASN			70.119	51.191	42.826	1.00 28.20		0
ATOM	1683	СВ	ASN			71.880	52.418	40.396	1.00 24.99		С
ATOM	1684	CG	ASN			72.642	51.980	39.163	1.00 26.53	•	С
ATOM	1685		ASN			72.333	50.943	38.572	1.00 25.64		0
ATOM	1686		ASN			73.650	52.756	38.774	1.00 24.62		N
									1.00 29.38		N
ATOM	1687	N	LYS			69.198	53.071	42.026			C
MOTA	1688	CA	LYS			68.545	53.410	43.276	1.00 30.78		
MOTA	1689	C	LYS			67.447	52.373	43.508	1.00 30.83		C
MOTA	1690	0	LYS			67.280	51.861	44.612	1.00 31.06		Ó
MOTA	1691	CB	LYS	A	344	67.947	54.810	43.172	1.00 33.74		C
ATOM	1692	CG	LYS	Α	344	67.298	55.335	44.437	1.00 38.78		C
MOTA	1693	CD	LYS	Α	344	66.906	56.799	44.255	1.00 41.30		C
MOTA	1694	CE	LYS	Α	344	66.250	57.364	45.501	1.00 43.10		C
ATOM	1695	NZ	LYS	A	344	65.928	58.810	45.325	1.00 46.21		N
ATOM	1696	N			345	66.715	52.054	42.448	1.00 29.99		N
ATOM	1697	CA			345	65.640	51.076	42.516	1.00 30.40		С
ATOM	1698	C			345	66.174	49.696	42.921	1.00 31.13		С
ATOM	1699	0			345	65.538	48.977	43.693	1.00 31.45		0
MOTA	1700	CB			345	64.950	50.968	41.162	1.00 29.11		C
							50.231	41.196	1.00 29.15		C
ATOM	1701	CG			345	63.630			1.00 29.67		C
ATOM	1702	CD1			345	62.465	50.880	41.597			C
MOTA	1703	CD2	TYR			63.539	48.896	40.802	1.00 28.37		
ATOM	1704		TYR			61.243	50.226	41.597	1.00 29.42		C
MOTA	1705		TYR			62.318		40.800	1.00 29.73		C
ATOM	1706	CZ			345	61.175	48.905	41.196			C
MOTA	1707	OH	TYR	Α	345	59.954	48.279		1.00 31.23		0
MOTA	1708	N	PHE	Α	346	67.334	49.328	42.387	1.00 31.61		N
MOTA	1709	CA	PHE	A	346	67.949	48.040	42.705	1.00 32.63		C
ATOM	1710	С	PHE	Α	346	68.288	47.958	44.194	1.00 33.80		C
MOTA	1711	0	PHE	Α	346	68.060	46.932	44.837	1.00 33.23		0
MOTA	1712	CB	PHE	Α	346	69.223	47.836	41.877	1.00 32.13		C
ATOM	1713	CG	PHE	Α	346	69.961	46.567	42.204	1.00 33.47		C
ATOM	1714		PHE			69.380	45.326	41.969	1.00 33.38		С
ATOM	1715		PHE			71.235	46.613	42.763	1.00 35.61		С
ATOM	1716		PHE			70.050	44.151	42.284	1.00 33.75		Ċ
							45.440	43.084	1.00 36.22		C
ATOM	1717		PHE			71.917			1.00 35.22		C
ATOM	1718	CZ			346	71.320	44.206	42.842			
ATOM	1719	N			347	68.826	49.045	44.737	1.00 34.63		N
MOTA	1720	CA			347	69.187	49.090	46.148	1.00 37.31		C
ATOM	1721	C			347	67.980	48.990	47.074	1.00 37.23		C
MOTA	1722	0	GLU	Α	347	68.068	48.393	48.144	1.00 38.77		0

ATOM	1723	CB	GLU	Δ	347	69.953	50.377	46.468	1.00	37.91			С
ATOM	1724	CG	GLU			71.349	50.441	45.877		43.97			C
		CD				72.215	49.262	46.296		47.61			C
MOTA	1725		GLU										0
MOTA	1726		GLU			72.231	48.923	47.501		50.24			
MOTA	1727					72.889	48.675	45.420		50.39			0
MOTA	1728	N	GLU			66.858	49.571	46.664		36.75		,	N
MOTA	1729	CA	GLU	Α	348	65.652	49.556	47.482		36.89			С
ATOM	1730	С	GLU	А	348	64.901	48.230	47.444	1.00	36.67	•		С
MOTA	1731	0	GLU	Α	348	64.376	47.780	48.460	1.00	37.48			0
MOTA	1732	CB	GLU	Α	348	64.672	50.643	47.022	1.00	37.65			C,
MOTA	1733	CG	GLU	A	348	65.295	51.969	46.635	1.00	40.22			С
ATOM	1734	CD	GLU	Α	348	64.265	52.960	46.108	1.00	40.32			С
ATOM	1735	OE1	GLU			63.309	52.526	45.434	1.00	41.11			0
ATOM	1736	OE2				64.417	54.174	46.356		41.33			0
ATOM	1737	N	THR			64.856	47.610	46.268		35.60			N
ATOM	1738	CA	THR			64.096	46.382	46.075		33.65			C
ATOM	1739	C	THR			64.859	45.094	45.759		33.57			C
		0	THR			64.282	44.006	45.807		33.25			0
MOTA	1740												C
ATOM	1741	CB	THR.			63.071	46.588	44.950		33.39			
MOTA	1742	OG1				63.763	46.710	43.700		32.24			0
ATOM	1743	CG2	THR			62.265	47.863	45.187		33.01			С
ATOM	1744	N	GLY			66.138	45.205	45.425		32.80			N
ATOM	1745	CA	GLY			66.903	44.018	45.085		31.46			С
ATOM	1746	C	GLY	Α	350	66.608	43.556	43.666		29.99			С
MOTA	1747	0	GLY	Α	350	67.073	42.503	43.232	1.00	30.31			0
MOTA	1748	N	ILE	Α	351	65.832	44.346	42.933	1.00	28.63			N
MOTA	1749	CA	ILE	Α	351	65.482	44.001	41.557	1.00	27.69			C
ATOM	1750	C	ILE	Α	351	66.327	44.807	40.575	1.00	27.05			C
ATOM	1751	0	ILE	Α	351	66.315	46.036	40.612	1.00	24.50			0
ATOM	1752	CB	ILE			64.004	44.315	41.253	1.00	29.37	,		С
ATOM	1753		ILE			63.092	43.640	42.281	1.00	31.00			С
ATOM	1754	CG2	ILE			63.662	43.862	39.841	1.00	28.85			С
ATOM	1755		ILE			61.625	44.051	42.154		32.57	,		Ç
ATOM	1756	N	TYR			67.060	44.121	39.702		26.80			N
ATOM	1757	CA			352	67.879	44.811	38.715		26.62			C
ATOM	1758	C	TYR			67.142	44.808	37.385		26.67			C
						66.899	43.751			26.28			0
ATOM	1759	O.	TYR					36.804 38.527		25.22			C
ATOM	1760	CB	TYR			69.240	44.130						
ATOM	1761	CG			352	70.153	44.886	37.578		24.08			C
ATOM	1762	CD1			352	70.961	45.931	38.035		22.64			C
MOTA	1763		TYR			70.185	44.580	36.218		23.85			C
MOTA	1764		TYR			71.780	46.647	37.161		21.59			C
MOTA	1765		TYR			70.998	45.294	35.334		22.91			C
MOTA	1766	CZ			352	71.793	46.321	35.814		21.43			С
MOTA	1767	OH	TYR	Α	352	72.621	47.001	34.951		22.44			0
ATOM	1768	N			353	66.782	45.992	36.906	1.00	26.51	•		N
MOTA	1769	CA	ILE	А	353	66.085	46.094	35.635	1.00	26.58			C
MOTA	1770	С	ILE	Α	353	67.019	46.605	34.542	1.00	26.72			C
ATOM	1771	0	ILE	Α	353	67.517	47.730	34.612	1.00	26.19			0
ATOM	1772	CB	ILE	А	353	64.882	47.042	35.735	1.00	27.79			С
ATOM	1773		ILE			63.948	46.566	36.855		28.55	•		С
MOTA	1774		ILE			64.147	47.086	34.399		27.23			С
ATOM	1775		ILE			62.751	47.446	37.089		27.39			C
ATOM	1776	N			354	67.290	45.770	33.526		25.87			N
ATOM	1777	CA			354	68.174	46.189	32.435		24.49			C
ATOM	1778	C			354	67.530	47.347	31.680		24.47			C
ATOM	1779	0			354	66.312	47.347	31.503		24.18			0
ATOM	1//3	Ų	PRO	A	3 5 tt	00.312	11.300	31.503	1.00	Z-1.10			J

ATOM	1780	CB	PRO	A	354	68.273	44.935	31.568	1.00	23.91			С
MOTA	1781	CG	PRO	Α	354	68.077	43.813	32.561	1.00	24.60			С
ATOM	1782	CD	PRO	Α	354	66.947	44.341	33.409	1.00	25.26			С
MOTA	1783	N	VAL	Α	355	68.333	48.317	31.250	1.00	23.40			N
ATOM	1784	CA	VAL	Α	355	67.783	49.433	30.495	1.00	22.64			C
ATOM	1785	C	VAL			68.418	49.464	29.119	1.00	22.19			С
ATOM	1786	0	VAL			69.576	49.090	28.944	1.00	21.72			0
ATOM	1787	CB	VAL.			67.989	50.805	31.211		23.23			С
ATOM	1788		VAL			67.314	50.773	32.582		20.89			С
ATOM	1789		VAL			69.478	51.144	31.325		20.18			С
ATOM	1790	N	CYS			67.640	49.905	28.141		21.94			N
ATOM	1791	CA			356 ·	68.100	49.965	26.769		22.63			C
	1792	C	CYS			68.172	51.393	26.251		23.07			C
ATOM						67.192	52.131	26.330		24.45			0
ATOM	1793	0	CYS				49.152	25.887		22.81			C
ATOM	1794	CB	CYS			67.148				23.52			s
ATOM	1795	SG	CYS			67.367	49.360	24.113		23.41			N
ATOM	1796	N			357	69.332	51.784	25.732					C
ATOM	1797	CA			357	69.480	53.118	25.158		23.70			
ATOM	1798	C			357	69.024	52.967	23.712		23.48			C
ATOM	1799	0			357	69.703	52.339	22.902		23.03			0
MOTA	1800	СВ			357	70.933	53.587	25.186		23.53			C
ATOM	1801	OG	SER	Α	357	71.039	54.865	24.579		23.13			0
ATOM	1802	N	ASP	Α	358	67.871	53.550	23.406		23.76			N
MOTA	1803	CA	ASP	Α	358	67.269	53.465	22.080		24.67			C
MOTA	1804	С	ASP	Α	358	67.363	54.754	21.268	1.00	25.27			С
MOTA	1805	0	ASP	A	358	66.749	55.762	21.608	1.00	24.49			0
ATOM.	1806	CB	ASP	Α	358	65.799	53.040	22.238	1.00	24.63		•	С
MOTA	1807	CG	ASP	Α	358	65.060	52.947	20.922	1.00	24.23			С
ATOM	1808	OD1	ASP			65.706	52.780	19.869	1.00	24.31			0
ATOM	1809		ASP			63.818	53.024	20.952	1.00	23.07			0
ATOM	1810	N			359	68.144	54.711	.20.192	1.00	26.85			N
ATOM	1811	CA			359	68.284	55.870	19.332	1.00	28.13			C
ATOM	1812	C			359	69.370	56.852	19.717		30.06			С
ATOM	1813	Ö			359	69.890	56.829	20.832		30.69			0
ATOM	1814	N			360	69.722	57.717	18.775		32.24			N
ATOM	1815	CA			360	70.740	58.714	19.037		34.39			С
MOTA	1816	C			360	72.159	58.243	18.804		34.76			C
		0			360	73.099	58.981	19.085		37.37			0
ATOM	1817				361	72.328	57.019	18.315		36.00			N
ATOM	1818	N				72.326	56.496			37.27			C
MOTA	1819	CA			361			16.627		39.44			C
ATOM	1820	C			361	74.052	56.893			39.25			0
ATOM	1821	0			361		56.392	15.657		36.74			C
MOTA	1822	CB			361		54.949	18.144					C
MOTA	1823		ILE			73.421	54.490	19.580		36.41			
MOTA	1824				361	75.081	54.442	17.679		35.82			C
MOTA	1825				361	74.512	54.788	20.589			•		C
MOTA	1826	N			362	75.024	57.793	16.508		41.13			N
MOTA	1827	CA			362	75.479	58.248	15.201		42.28			C
MOTA	1828	C	VAL	A	362	76.807	57.608	14.801		42.57			С
MOTA	1829	0	VAL	A	362	76.993	57.249	13.640		44.09			0
MOTA	1830	CB	VAL	A	362	75.630	59.781	15.167		43.37			C
MOTA	1831	CG1	VAL	A	362	76.025	60.236	13.762	1.00	44.64			C
MOTA	1832	CG2	VAL	Α	362	74.324	60.438	15.592	1.00	43.73			C
MOTA	1833	N	TYR	A	363	77.722	57.459	15.760	1.00	41.34			N
MOTA	1834	CA			363	79.032	56.857	15.495	1.00	39.51			С
ATOM	1835	С			363		55.654	16.396	1.00	37.48			С
ATOM	1836	0			363	78.654	55.512	17.440		37.25			0

ATOM	1837	CB	TYR	A	363	80.136	57.887	15.718	1.00 41.87		С
MOTA	1838	CG	TYR	Α	363	79.974	59.140	14.896	1.00 45.48		С
MOTA	1839	CD1	TYR	A	363	80.011	59.093	13.504	1.00 47.49		C
ATOM	1840	CD2	TYR	Α	363	79.779	60.374	15.509	1.00 46.57		С
MOTA	1841	CE1	TYR	Α	363	79.858	60.246	12.742	1.00 49.35		С
MOTA	1842	CE2			363	79.625	61.531	14.759	1.00 48.79		C
ATOM	1843	CZ			363	79.666	61.461	13.377	1.00 49.83		C
ATOM	1844	ОН			363	79.519	62.610	12.629	1.00 52.64		0
ATOM	1845	N			364	80.223	54.793	16.007	1.00 35.17		N
ATOM	1846	CA			364	80.523	53.619	16.821	1.00 34.10		C
ATOM	1847	C			364	80.846	53.973	18.271	1.00 32.20		C
ATOM	1848	0			364	80.387	53.298	19.191	1.00 32.20		0
ATOM	1849	СВ			364	81.696	52.815	16.240	1.00 35.00		C
ATOM	1850	CG			364	81.321	52.013	14.991	1.00 36.21		C
ATOM	1851		ASP			80.170	51.566	14.885	1.00 36.58		0
ATOM	1852		ASP			82.194	51.860	14.118	1.00 38.57		0
ATOM		N									
	1853				365	81.621	55.033	18.485	1.00 30.02		N
MOTA	1854	CA			365	81.994	55.401	19.848	1.00 28.95		C
ATOM	1855	C			365	80.802	55.809	20.709	1.00 27.94		C
ATOM	1856	0			365	80.899	55.825	21.931	1.00 26.36		0
ATOM .	1857	CB			365	83.081	56.489	19.843	1.00 28.15		C
ATOM	1858	CG			365	82.607	57.921	19.696	1.00 29.09		C
ATOM	1859		TYR			82.405	58.729	20.816	1.00 28.03		С
MOTA	1860		TYR			82.421	58.487	18.437	1.00 29.60		С
MOTA	1861	CE1				82.039	60.073	20.681	1.00 29.32	•	C
ATOM	1862	CE2	TYR			82.055	59.830	18.291	1.00 30.03		С
ATOM	1863	CZ			365	81.868	60.613	19.414	1.00 30.20		C
ATOM	1864	OH			365	81.519	61.936	19.259	1.00 32.66		0
MOTA	1865	N	HIS			79.674	56.126	20.074	1.00 28.10		N
MOTA	1866	CA	HIS	A	366	78.478	56.477	20.829	1.00 27.17	•	С
ATOM	1867	С	HIS	A	366	77.995	55.216	21.548	1.00 25.93		С
MOTA	1868	0	HIS	Α	366	77.380	55.301	22.609	1.00 24.73		0
MOTA	1869	CB	HIS	Α	366	77.371	57.003	19.909	1.00 28.22		С
ATOM	1870	CG	HIS	Α	366	77.616	58.387	19.394	1.00 29.65		C
MOTA	1871	ND1	HIS	Α	366	78.642	59.184	19.856	1.00 31.11		N
MOTA	1872	CD2	HIS	Α	366	76.947	59.129	18.481	1.00 30.20		C
MOTA	1873	CE1	HIS	Α	366	78.593	60.357	19.252	1.00 29.57		С
MOTA	1874	NE2	HIS	Α	366	77.574	60.350	18.412	1.00 31.07		N
MOTA	1875	N	MET	A	367	78.275	54.051	20.960	1.00 24.23		N
MOTA	1876	CA	MET	A	367	77.892	52.773	21.569	1.00 24.28		C
ATOM	1877	C	MET	A	367	78.634	52.627	22.892	1.00 22.96		С
MOTA	1878	0	MET	Α	367	78.036	52.342	23.924	1.00 23.44		0
MOTA	1879	CB	MET	Α	367	78.273	51.595	20.666	1.00 24.50		С
MOTA	1880	CG	MET	Α	367	77.537	51.530	19.332	1.00 26.42		С
ATOM	1881	ŞD	MET	А	367	78.087	50.102	18.355	1.00 29.45		s
MOTA	1882	CE	MET			77.053	50.267	16.894	1.00 28.05		C
MOTA	1883	N			368	79.947	52.827	22.853	1.00 23.22		N
ATOM	1884	CA	THR			80.764	52.719	24.058	1.00 23.72		C
MOTA	1885	C	THR			80.266	53.711	25.110	1.00 22.92		C
ATOM	1886	Ö	THR			80.180	53.379	26.290	1.00 23.78		0
ATOM	1887	СВ	THR			82.249	53.005	23.748	1.00 24.12		C
MOTA	1888		THR			82.625	52.305	22.554	1.00 24.48		0
ATOM	1889		THR			83.138	52.537	24.902	1.00 23.20		C
ATOM	1890	N	LEU			79.939	54.929	24.680	1.00 23.20		N
ATOM	1891	CA	LEU			79.435	55.947	25.602	1.00 22.01		C
ATOM	1892	C	LEU			78.125	55.525	26.253	1.00 22.78		C
MOTA	1893	0	LEU			77.958	55.659				0
771 014	1023	0	ייביי	7-7	202	11.330	25.653	27.464	1.00 23.15		Ų

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MOTA	1894	СВ	LEU .	Α	369	79.217	57.280	24.882	1.00 21.96		С
MOTA	1895	CG	LEU .	A	369	80.456	58.127	24.604	1.00 23.46		C
MOTA	1896	CD1	LEU .	A	369	80.050	59.369	23.807	1.00 22.62		C
MOTA	1897	CD2	LEU .	Α	369	81.114	58.520	25.929	1.00 21.25		C
MOTA	1898	N	ALA .	Α	370	77.197	55.016	25.445	1.00 21.89		N
MOTA	1899	CA	ALA	Α	370	75.898	54.592	25.956	1.00 22.53		С
ATOM	1900	С	ALA	Α	370	76.069	53.503	27.013	1.00 21.32		С
MOTA	1901	0	ALA	Α	370	75.411	53.524	28.047	1.00 22.46		0
MOTA	1902	CB	ALA	Α	370	75.018	54.087	24.805	1.00 20.75		С
MOTA	1903	N	LEU	Α	371	76.959	52.555	26.751	1.00 21.38		N
ATOM	1904	CA	LEU	A	371	77.205	51.470	27.693	1.00 21.60		C
ATOM	1905	C	LEU	Α	371	77.899	52.010	28.950	1.00 22.18		С
MOTA	1906	0	LEU	Α	371	77.494	51.700	30.063	1.00 22.86		0
ATOM	1907	CB	LEU	Α	371	78.062	50.384	27.029	1.00 20.20		C
ATOM	1908	CG	LEU	Α	371	77.444	49.692	25.806	1.00 21.57		C
ATOM	1909	CD1	LEU	Α	371	78.482	48.784	25.147	1.00 23.83		С
MOTA	1910	CD2	LEU	Α	371	76.220	48.884	26.228	1.00 21.62		C
MOTA	1911	N	ALA	Α	372	78.932	52.835	28.763	1.00 22.30		N
MOTA	1912	CA	ALA	Α	372	79.675	53.407	29.883	1.00 22.28		C
	1913	. C	ALA	Α	372	78.768	54.196	30.814	1.00 23.49		C
ATOM	1914	0	ALA	A	372	78.979	54.225	32.027	1.00 22.49		0
ATOM	1915	CB	ALA	А	372	80.794	54.305	29.369	1.00 21.55		С
ATOM	1916	N	MET	Α	373	77.763	54.848	30.242	1.00 23.46		N
MOTA	1917	CA	MET	Α	373	76.837	55.631	31.043	1.00 23.37		С
ATOM	1918	C	MET	Α	373	75.850	54.762	31.830	1.00 22.64		С
MOTA	1919	0	MET	Α	373	75.111	55.269	32.662	1.00 22.93		0
MOTA	1920	CB	MET	A	373	76.100	56.639	30.150	1.00 23.08		С
MOTA	1921	CG	MET	А	373	77.007	57.763	29.640	1.00 23.17		С
ATOM	1922	SD	MET	Α	373	76.206	58.901	28.474	1.00 23.90		S
MOTA	1923	CE	MET	Α	373	77.545	60.031	28.102	1.00 22.19		C
MOTA	1924	N	GLY	Α	374	75.842	53.457	31.577	1.00 23.01		N
MOTA	1925	CA	GLY	Α	374	74.952	52.579	32.322	1.00 22.40		C
MOTA	1926	С	GLY	А	374	73.945	51.751	31.540	1.00 23.47		С
MOTA	1927	0	GLY	Α	374	73.316	50.853	32.106	1.00 24.05		0
MOTA	1928	N	ALA	Α	375	73.764	52.041	30.257	1.00 22.06		N
MOTA	1929	CA	ALA	Α	375	72.826	51.264	29.460	1.00 23.47		С
MOTA	1930	C	ALA	Α	375	73.365	49.840	29.331	1.00 23.69		С
MOTA	1931	0	ALA	Α	375	74.549	49.641	29.065	1.00 25.05		0
MOTA	1932	CB	ALA	Α	375	72.655	51.887	28.082	1.00 20.67		C
ATOM	1933	N	ASP	Α	376	72.497	48.854	29.528	1.00 24.20		N
ATOM	1934	CA	ASP	Α	376	72.895	47.453	29.431	1.00 24.16		C
ATOM	1935	C	ASP	Α	376	73.021	47.053	27.968	1.00 23.81		C
MOTA	1936	0	ASP	A	376	73.937		27.596	1.00 23.82		0
MOTA	1937	CB	ASP	A	376	71.878		30.159	1.00 24.02		C
MOTA	1938	CG	ASP	Α	376	71.763		31.632	1.00 24.67		C
MOTA	1939	OD1	ASP	A	376	72.561		32.444	1.00 24.99		0
MOTA	1940	OD2	ASP			70.889		31.977	1.00 24.71		0
MOTA	1941	N			377	72.094		27.139	1.00 23.81		N
MOTA	1942	`CA	PHE	A	377	72.164		25.712	1.00 23.63		C
MOTA	1943	C			377	71.667		24.905	1.00 23.27		C
MOTA	1944	0	PHE	A	377	71.132		25.462	1.00 22.71		0
MOTA	1945	CB			377	71.427		25.320	1.00 22.50		C
MOTA	1946	CG			377	70.013		25.817	1.00 23.64		C
MOTA	1947		PHE			69.748		27.132	1.00 25.15		C
MOTA	1948		PHE			68.941		24.953	1.00 22.89		C
MOTA	1949		PHE			68.428		27.579	1.00 25.01		C
MOTA	1950	CE2	PHE	A	. 377	67.626	45.895	25.387	1.00 23.60		С

ATOM	1951	CZ	PHE	Α	377	67.369	45.516	26.702	1.00	24.96		С
MOTA	1952	N	ILE	A	378	71.857	48.376	23.592	1.00	22.99		N
MOTA	1953	CA	ILE	A	378	71.512	49.470	22.698	1.00	23.32		С
MOTA	1954	С	ILE	A	378 .	70.573	49.043	21.573	1.00	24.13		С
ATOM	1955	0	ILE	A	378	70.760	47.983	20.978	1.00	24.04		0
MOTA	1956	CB	ILE	Α	378	72.815	50.030	22.061	1.00	24.07		C
ATOM	1957	CG1			378	73.807	50.406	23.163	1.00	25.55		С
ATOM	1958	CG2	ILE			72.521	51.232	21.176		23.97.		С
ATOM	1959	CD1	ILE			75.242	50.486	22.665		25.45		C
ATOM	1960	N	MET			69.565	49.866	21.285		23.06		Ŋ
ATOM	1961	CA	MET			68.643	49.566	20.195		23.94		C
ATOM	1962	C			379	68.968	50.516	19.045		24.07		C
ATOM	1963	0	MET			69.061	51.725	19.237		23.67		0
										23.89		C
ATOM	1964	CB	MET			67.179	49.746	20.621				
ATOM	1965	CG	MET			66.206	49.546	19.461		23.47		'C
ATOM	1966	SD	MET			64.466	49.424	19.913		23.78		S.
ATOM	1967	CE	MET			64.375	47.682	20.458		23.21		C
MOTA	1968	N	LEU			69.136	49.961	17.851		24.45		N
MOTA	1969	CA	LEU		380	69.476	50.758	16.682		25.64		С
ATOM	1970	С	LEU	A	380	68.561	50.484	15.502		25.46		C
MOTA	1971	0	LEU	Α	380	68.162	49.346	15.265	1.00	24.86		0
MOTA	1972	CB	LEU	Α	380	70.922	50.477	16.259	1.00	26.84		C
ATOM	1973	CG	LEU	Α	380	72.033	50.818	17.255	1.00	28.40		C
MOTA	1974	CD1	LEU	Α	380	73.394	50.462	16.689	1.00	28.92		C
MOTA	1975	CD2	LEU	Α	380	71.977	52.299	17.546	1.00	31.59		C
ATOM	1976	N	GLY	Α	381	68.238	51.539	14.764	1.00	26.35		N
MOTA	1977	CA	GLY	A	381	67.398	51.397	13.587	1.00	27.38		C
MOTA	1978	C	GLY	Α	381	68.230	51.618	12.335	1.00	27.51		C
MOTA	1979	0	GLY	Α	381	68.535	50.679	11.604	1.00	27.02		0
ATOM	1980	N	ARG			68.611	52.870	12.108	1.00	29.52		N
MOTA	1981	CA	ARG			69.412	53.264	10.947	1.00	32.19		C.
MOTA	1982	С	ARG			70.626	52.353	10.722	1.00	30.92		C
MOTA	1983	0	ARG			70.878	51.899	9.608	1.00	30.21		0
ATOM	1984	CB	ARG			69.895	54.707	11.125		35.86		C
ATOM	1985	CG	ARG			69.994	55.497	9.834		42.94		.C
ATOM	1986	CD	ARG			70,799	56.793	9.990		48.04		C
MOTA	1987	NE			382	72.237	56.531	10.060		52.92		N
ATOM	1988	CZ			382	72.883	56.136	11.156		55.81		C
ATOM	1989	NH1	ARG			72.228	55.961	12.296				N
ATOM	1990	NH2				74.187	55.896	11.106		56.34		N
	1991						52.105	11.791		29.98		N
MOTA		N			383 383	71.376		11.748		28.39		C
ATOM	1992	CA				72.569	51.261					C
ATOM	1993	C			383	72.324	49.926	11.034		28.21		
MOTA	1994	0			383	73.084	49.543	10.143		27.77		0
ATOM	1995	CB	TYR			73.059	51.000	13.179		26.48		C
ATOM	1996	CG			383	74.301	50.137	13.276		25.37	-	C
MOTA		CD1				75.578	50.703	13.240		24.67		C
MOTA	1998		TYR			74.196	48.752	13.397		24.26		С
MOTA	1999		TYR			76.716	49.910	13.322		24.73		C
ATOM	2000	CE2			. 383	75.320	47.951	13.479		23.84		C
MOTA	2001	CZ			383	76.578	48.530	13.440		25.89		C
MOTA	2002	OH			383	77.689	47.722	13.511		25.39		0
MOTA	2003	N			384	71.263	49.228	11.428		27.07		N
MOTA	2004	CA			384	70.922	47.931	10.843		28.18		С
ATOM	2005	C			384	70.200	48.007	9.493		28.50		С
MOTA	2006	0			384	70.278	47.076	8.696		29.39		0
MOTA	2007	CB.	PHE	A	384	70.068	47,122	11.827	1.00	25.94		С

ATOM	2008	CG	PHE	Α	384	70.832	46.611	13.025	1.00 26.50		С
ATOM	2009	CD1	PHE	Α	384	71.790	45.610	12.882	1.00 25.77		С
ATOM	2010	CD2	PHE	Α	384	70.595	47.133	14.295	1.00 25.04		C
MOTA	2011	CE1	PHE	Α	384	72.502	45.135	13.983	1.00 25.85		С
ATOM	2012	CE2	PHE	Α	384 .	71.300	46.666	15.402	1.00 26.26		С
ATOM	2013	CZ	PHE	A	384	72.258	45.663	15.246	1.00 25.10		C
ATOM	2014	N	ALA			69.493	49.105	9.244	1.00 29.51		N
ATOM	2015	CA			385	68.758	49.281	7.996	1.00 29.99		С
ATOM	2016	С			385	69.686	49.249	6.780	1.00 31.15		C
ATOM	2017	o			385	69.275	48.868	5.685	1.00 31.07		0
ATOM	2018	СВ			385	67.993	50.600	8.033	1.00 29.53		C
ATOM	2019	N			386	70.939	49.647	6.989	1.00 23.33		N
ATOM	2020	CA			386	71.949	49.686	5.936	1.00 32.12		C
ATOM	2020	C			386	72.391		5.453	1.00 32.14		C
							48.308				0
ATOM	2022	0			386	72.983	48.180	4.380	1.00 33.24		C
ATOM	2023	CB			386	73.204	50.405	6.434	1.00 32.61		
ATOM	2024	CG			386	73.039	51.825	6.908	1.00 33.83		C
ATOM	2025	CD			386	74.356	52.269	7.538	1.00 36.13		C
MOTA	2026	NE			386	74.740	51.371	8.628	1.00 36.98		N
MOTA	2027	CZ.	ARG			75.990	51.156	9.027	1.00 37.29		Ç
ATOM	2028		ARG			77.004	51.772	8.429	1.00 36.98		N
ATOM	2029	NH2	ARG			76.227	50.318	10.027	1.00 36.19		N
MOTA	2030	N			387	72.126	47.279	6.248	1.00 33.19		N
MOTA	2031	CA			387	72.565	45.941	5.890	1.00 33.56		C
MOTA	2032	C	PHE	А	387	71.710	45.194	4.872	1.00 35.13		С
ATOM	2033	0	PHE	Α	387	70.511	45.448	4.711	1.00 34.37		0
ATOM	2034	CB	PHE	A	387	72.725	45.085	7.155	1.00 32.86		C
MOTA	2035	ÇG	PHE	Α	387	73.621	45.701	8.200	1.00 32.36		C
ATOM	2036	CD1	PHE	А	387	74.756	46.417	7.832	1.00 31.61		C
MOTA	2037	CD2	PHE	Α	387	73.331	45.563	9.553	1.00 31.75		C
ATOM	2038		PHE			75.586	46.991	8.797	1.00 32.70		С
MOTA	2039	CE2	PHE	Α	387	74.156	46.132	10.529	1.00 31.49		C
ATOM	2040	CZ			387	75.284	46.848	10.151	1.00 30.49		С
ATOM.	2041	N			388	72.364	44.265	4.186	1.00 35.81		N
ATOM	2042	CA			388	71.731	43.428	3.181	1.00 36.15		C
ATOM	2043	C			388	70.509	42.735	3.770	1.00 34.62		C
ATOM	2044	Ö			388	69.494	42.577	3.098	1.00 33.35		0
ATOM	2045	СВ			388	72.730	42.374	2.689	1.00 38.38		C
MOTA	2046		GLU			72.730	41.319	1.771	1.00 30.30		C
ATOM	2047	CD			388	72.130	41.870	0.404	1.00 45.98	•	C
ATOM	2048				388.	70.997	41.216	-0.324	1.00 48.50		0
ATOM	2049		GLU			72.297	42.954	0.054	1.00 47.51		0
ATOM	2050	N			389	70.609	42.343	5.038	1.00 33.73	-	N
ATOM	2051	CA			389	69.526	41.639	5.706	1.00 33.32		C
ATOM	2052	C			389	68.295	42,448	6.115	1.00 33.33		C
ATOM	2053	0			389	67.313	41.864	6.563	1.00 33.97		0
MOTA	2054	CB			389	70.067	40.883	6.924	1.00 33.42		С
MOTA	2055	CG			389	71.099	39.827	6.575	1.00 33.24		С
MOTA	2056	CD			389	72.525	40.343	6.656	1.00 34.22		C
MOTA	2057		GLU			72736	41.563	6.511	1.00 33.67		0
MOTA	2058	OE2	GLU			73.441	39.519	6.854	1.00 34.50	•	0
MOTA	2059	N	SER	Α	390	68.328	43.772	5.986	1.00 33.75		N
MOTA	2060	CA	SER	A	390	67.145	44.558	6.341	1.00 35.12		C
MOTA	2061	С .	SER	Α	390	66.106	44.264	5.252	1.00 36.23		С
ATOM	2062	0	SER	A	390	66.462	44.028	4.097	1.00 35.59		0
MOTA	2063	CB			390	67.456	46.055	6.397	1.00 33.40		C
MOTA	2064	OG			390	67.716	46.575	5.112	1.00 35.26		0
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A TOM	2065	NT.	חחח	70.	201	C4 013	44 200	E (00	1 00	37 60			N.T
MOTA	2065	N	PRO			64.811	44.290	5.608		37.69			N
MOTA	2066	CA	PRO			63.704	44.012	4.686		39.43	•		С
MOTA	2067	C	PRO			63.332	45.059	3.635	1.00	40.72			С
MOTA	2068	0	PRO	A	391	62.291	44.938	2.991	1.00	41.37			0
MOTA	2069	CB	PRO	А	391	62.548	43.729	5.639	1.00	39.02			С
MOTA	2070	CG	PRO	Α	391	62.797	44.733	6.725	1.00	38.46			C
MOTA	2071	CD	PRO	Α	391	64.300	44.637	6.949	1.00	36.88			С
MOTA	2072	N	THR			64.167	46.071	3.443		41.57			N
ATOM	2073	CA	THR			63.844	47.103	2.469		42.35			C
ATOM	2074	C	THR			64.520	46.929	1.114		44.91			C
ATOM	2075	0	THR			65.399	46.084	0.938		45.02			
													0
MOTA	2076	CB	THR			64.178	48.502	3.011		41.05			C
MOTA	2077	OG1	THR			65.579	48.587	3.293		39.97			0
MOTA	2078	CG2	THR			63.383	48.778	4.281		39.92			С
ATOM	2079	N	ARG	A	393 .	64.094	47.747	0.159	1.00	47.45			N
MOTA	2080	CA	ARG	Α	393	64.623	47.703	-1.195	1.00	50.03			C
MOTA	2081	C	ARG	Α	393	65.990	48.355	-1.317	1.00	50.45			С
MOTA	2082	0	ARG	Α	393	66.243	49.419	-0.751	1.00	50.27			0
MOTA	2083	CB	ARG			63.640	48.380	-2.163	1.00	51.81			С
ATOM	2084	CG	ARG			62.377	47.565	-2.431		54.92			C
ATOM	2085	CD	ARG			61.284	48.366	-3.146		57.32			C
ATOM	2086	NE	ARG			61.775							
							49.068	-4.328		59.58			N
ATOM	2087	CZ	ARG			62.024	50.375	-4.370		61.26			C
MOTA	2088		ARG			61.823	51.125	-3.295		61.47			N
MOTA	2089		ARG			62.481	50.934	-5.484		62.64			N
ATOM	2090	N	LYS	A	394	66.872	47.690	-2.053	1.00	50.90			N
MOTA	2091	CA	LYS			68.213	48.191	-2.299	1.00	51.87			С
MOTA	2092	С	LYS	Α	394	68.046	49.050	-3.545	1.00	53.29			С
MOTA	2093	0	LYS	A	394	67.637	48.551	-4.590	1.00	53.60			0
MOTA	2094	CB	LYS	A	394	69.158	47.023	-2.579	1.00	51.11			С
ATOM	2095	CG	LYS			70.618	47.333	-2.352	1.00	50.68			C
ATOM	2096	CD	LYS			71.508	46.184	-2.795		49.41			C
MOTA	2097	CE	LYS			71.231	44.910	-2.025		48.96			C
MOTA	2098	NZ	LYS			72.139	43.816	-2.476		47.88			N
MOTA	2099	N	VAL			68.343	50.340			55.26			
								-3.435					N
MOTA	2100	CA	VAL			68.183	51.253	-4.562		57.43		,	C
ATOM	2101	C	VAL			69.475	51.939	-4.979		58.81			С
MOTA	2102	0	VAL			70.207	52.463	-4.145		59.36			0
MOTA	2103	CB	VAL			67.141	52.344	-4.238		57.67			С
MOTA	2104	CG1	VAL	A	395	67.047	53.339	-5.388		58.68			C
MOTA	2105	CG2	VAL	Α	395	65.789	51.703	-3.974	1.00	57.82			С
MOŢA	2106	N	THR	Α	396	69.740	51.946	-6.281	1.00	60.52			N
MOTA	2107	CA	THR	A	396	70.942	52.577	-6.813	1.00	62.17			C
ATOM	2108	С	THR	Α	396	70.648	53.995	-7.284	1.00	63.08			С
MOTA	2109	0	THR			69.919	54.197	-8.255		63.34			0
MOTA	2110	СВ	THR			71.514	51.781	-7.998		62.45			С
ATOM	2111		THR			71.837	50.454	-7.569		63.27			ō
ATOM	2112		THR			72.772	52.452	-8.529		63.24			C
ATOM	2113	N	ILE			71.222	54.970	-6.586		64.02			И
ATOM	2114	CA	ILE			71.035	56.376	-6.918		65.04			C
ATOM	2115	C	ILE			72.365	56.980	-7.362		65.43			C
MOTA	2116	0	ILE			73.287	57.134	-6.559		65.88			0
ATOM	2117	CB	ILE			70.509	57.168	-5.701	1.00	65.43			С
MOTA	2118	CG1	ILE	Α	397	69.229	56.516	-5.171	1.00	65.85			Ċ
ATOM	2119		ILE			70.230	58.608	-6.099	1.00	65.50			С
MOTA	2120	CD1	ILE	A	397	68.688	57.167	-3.914	1.00	66.46			С
ATOM	2121	N	ASN			72.450	57.319	-8.644	1.00	65.44			N

ATOM	2122	CA	ASN	A	398	73.652	57.900	-9.238	1.00 65.1	3		С
MOTA	2123	C	ASN	А	398	74.959	57.251	-8.770	1.00 63.5	9		C
MOTA	2124	0	ASN	A	398	75.819	57.911	-8.186	1.00 63.1	3		0
MOTA	2125	CB	ASN	A	398	73.703	59.417	-8.988	1.00 67.2	6		C
MOTA	2126	CG	ASN	А	398	73.838	59.773	-7.515	1.00 69.2	0		С
MOTA	2127	OD1	ASN	Α	398	72.906	59.598	6.730	1.00 70.2	1		0
ATOM	2128	ND2	ASN	Α	398	75.009	60.278	-7.135	1.00 69.8			N
MOTA	2129	N	GLY	A	399	75.097	55.954	-9.031	1.00 61.7	0		N
ATOM	2130	CA	GLY	A	399	76.306	55.242	-8.653	1.00 59.4			С
ATOM	2131	C	GLY			76.406	54.789	-7.207	1.00 57.8			С
ATOM	2132	0	GLY			77.324	54.047	-6.850	1.00 57.9			0
MOTA	2133	Ν.			400	75.477	55.232	-6.368	1.00 55.7			N
ATOM	2134	CA			400	75.495	54.850	-4.960	1.00 52.8			C
MOTA	2135	С			400	74.343	53.929	-4.604	1.00 50.5			C
ATOM	2136	0			400	73.182	54.249	-4.841	1.00 50.8			0
MOTA	2137	CB			400	75.445	56.090	-4.067	1.00 52.3			C
MOTA	2138	OG			400	76.657	56.816	-4.147	1.00 53.5			0
MOTA	2139	N			401	74.672	52.778	-4.033	1.00 48.1			N
MOTA	2140	CA			401	73.655	51.824	-3.629	1.00 46.0			C
MOTA	2141	C			401	73.166	52.225	-2.237	1.00 45.5			C
MOTA	2142	0			401	73.959		1.302 .				0
ATOM	2143	CB			401	74.224	50.397	-3.605	1.00 45.6			C
MOTA	2144		VAL			73.149	49.412	-3.178	1.00 44.5			C
ATOM	2145		VAL			74.768	50.041	-4.985	1.00 44.6		,	C
ATOM	2146	N			402	71.856	52.418	-2.118	1.00 44.6			N
ATOM	2147	CA			402	71.236	52.829	-0.863	1.00 43.4			C
ATOM	2148	C			402	70.154	51.846	-0.434				C
ATOM	2149	0			402	69.786	50.933	-1.175	1.00 41.1			0
ATOM	2150	CB			402	70.580	54.208	-1.020	1.00 45.1			C
ATOM	2151	CG			402	71.414	55.261	-1.728	1.00 45.4			C S
ATOM	2152	SD			402	72.814	55.813	-0.761	1.00 50.4			C
ATOM	2153	CE			402	72.042	57.060	0.274	1.00 47.0 1.00 40.2			N
ATOM	2154	N			403	69.646	52.045	0.776	1.00 40.2			C
ATOM	2155 2156	CA - C			403	68.575 67.506	51.217	1.297 1.827	1.00 38.8			C
ATOM		0			403 403	67.805	52.157	2.325	1.00 37.8			0
ATOM ATOM	2157 2158	CB			403	69.071	53.246 50.295	2.323	1.00 37.8			C
ATOM	2159	CG			403	70.049	49.234	1.944	1.00 38.1			C
ATOM	2160	CD			403	69.733	47.871	2.535	1.00 38.4			c
MOTA	2161	CE			403	68.425	47.321	1.989	1.00 38.2			C
ATOM	2162	NZ		-	403		45.957		1.00 36.2			N
ATOM	2163	N			404	•	51.746	1.697	1.00 39.2		•	N
ATOM	2164	CA			404		.52.567	2.169	1.00 39.4			C
ATOM	2165	C			404	65.108	52.518	3.682	1.00 38.8			C
ATOM	2166	0			404	65.459	51.509	4.297	1.00 37.6			0
ATOM	2167	CB			404	63.840	52.060	1.609	1.00 41.5			C
ATOM	2168	CG			404	63.763	52.059	0.103	1.00 45.3			C
ATOM	2169	CD			404	62.435	51.539	-0.384	1.00 46.1			C
ATOM	2170				404	62.155	50.338	-0.167	1.00 47.8			0
ATOM	2171				404	61.673	52.334	-0.971	1.00 47.6			0
ATOM	2172	N			405	64.665	53.616	4.275	1.00 38.0			N
ATOM	2173	CA			405	64.550	53.700	5.717	1.00 37.6			С
ATOM	2174	C			405	63.512	54.746	6.066	1.00 36.9			C
ATOM	2175	Ō			405	63.619	55.899	5.658	1.00 37.9			0
MOTA	2176	СВ			405	65.892	54.078	6.335	1.00 37.4			С
MOTA	2177	CG			405	65.857	54.147	7.842	1.00 37.4			С
MOTA	2178				405	65.593	53.013	8.603	1.00 36.2			C

MOTA	2179	CD2	TYR	Α	405	66.084	55.349	8.507	1.00 38.07		С
MOTA	2180	CE1	TYR	Α	405	65.557	53.072	9.990	1.00 36.68		С
ATOM	2181	CE2	TYR	A	405	66.049	55.417	9.892	1.00 38.81		С
ATOM	2182	CZ	TYR	Α	405	65.784	54.274	10.627	1.00 36.81		C
ATOM	2183	OH	TYR	Α	405	65.736	54.345	11.999	1.00 37.95		0
MOTA	2184	N	TRP			62.498	54.336	6.813	1.00 35.74		N
ATOM	2185	CA	TRP			61.450	551256	7.214	1.00 34.25		C
ATOM	2186	C	TRP			61.075	54.979	8.661	1.00 34.05		C
ATOM	2187	0	TRP			61.165	53.841	9.126	1.00 33.82		0
ATOM	2188	CB	TRP			60.232	55.113	6.281	1.00 32.23		C
ATOM	2189	CG	TRP			59.577	53.763	6.285	1.00 32.23		C
	2190					58.605		7.138	1.00 29.14		C
ATOM		CD1	TRP				53.327		1.00 29.14		C
ATOM	2191					59.874	52.659	5.419			
ATOM	2192		TRP			58.280	52.023	6.860	1.00 28.25		N
ATOM	2193	CE2	TRP			59.045	51.586	5.811	1.00 28.80		C
ATOM	2194		TRP			60.764	52.472	4.350	1.00 30.06		C
ATOM	2195	CZ2	TRP			59.077	50.337	5.173	1.00 29.23		C
MOTA	2196	CZ3	TRP			60.797	51.230	3.713	1.00 30.49		С
MOTA	2197		TRP			59.956	50.178	4.131	1.00 30.09		C
MOTA	2198	N	GLY			60.682	56.030	9.372	1.00 33.97		N
MOTA	2199	CA	GLY			60.300	55.883	10.763	1.00 35.09		C
MOTA	2200	C	GLY	Α	407	58.921	55.270	10.912	1.00 35.29		C
MOTA	2201	0	GLY	A	407	58.124	55.281	9.978	1.00 34.78		0
MOTA	2202	N	GLU	Α	408	58.640	54.723	12.090	1.00 35.40		N
MOTA	2203	CA	GLU	Α	408	57.347	54.112	,12.356	1.00 35.13		C
MOTA	2204	C	GLU	A	408	56.273	55.189	12.468	1.00 36.19		C
MOTA	2205	0	GLU	Α	408	55.081	54.899	12.408	1.00 35.83		0
MOTA	2206	CB	GLU	A	408	57.414	53.295	13.647	1.00 33.46		C
MOTA	2207	CG	GLU	A	408	58.193	51.999	13.498	1.00 32.80		С
MOTA	2208	CD	GLU			57.499	51.006	12.569	1.00 31.60		С
MOTA	2209	ÓE1				56.402	50.534	12.918	1.00 29.78		0
ATOM	2210		GLU			58.047	50.701	11.490	1.00 31.44	•	0
ATOM	2211	N	GLY			56.709	56.436	12.619	1.00 37.77		N
MOTA	2212	CA	GLY			55.773	57.539	12.734	1.00 39.49		C
MOTA	2213	C	GLY			55.400	58.156	11.397	1.00 40.71		C
ATOM	2214	Ō	GLY			54.482	58.970	11.323	1.00 40.61		0
MOTA	2215	N	SER			56.109	57.782	10.338	1.00 42.27		N
MOTA	2216	CA	SER			55.813	58.318	9.013	1.00 42.27		C
								8.526			C
ATOM	2217	C	SER			54.485	57.742		1.00 45.74		
MOTA	2218	0	SER			54.065	56.672	8.968	1.00 44.79 1.00 43.45		0
MOTA	2219	CB			410	56.917	57.952	8.017			_
MOTA	2220	OG			410		`56.587	7.641	1.00 44.08		0
MOTA	2221	. И			411	53.828	58.457	7.618	1.00 48.17		N
MOTA	2222	CA			411	52.556	57.998	7.081	1.00 50.72		C
MOTA	2223	С			411	52.777	56.708	6.301	1.00 51.98		C
MOTA	2224	0			411	51.885	55.865	6.205	1.00 51.95		0
MOTA	2225	CB			411	51.947	59.064	6.170	1.00 51.02		C
MOTA	2226	OG	SER	A	411	52.832	59.393	5.116	1.00 52.23		0
MOTA	2227	N	ARG	A	412	53.978	56.555	5.754	1.00 53.68		N
MOTA	2228	CA	ARG	A	412	54.323	55.363	4.989	1.00 55.96		C
MOTA	2229	C	ARG	A	412	54.226	54.083	5.819	1.00 58.17		C
MOTA	2230	0	ARG	Α	412	54.018	53.000	5.275	1.00 57.86		0
MOTA	2231	CB			412	55.741	55.491	4.419	1.00 54.66		C
MOTA	2232	CG	ARG	Α	412	56.208	54.242	3.687	1.00 53.34		C
ATOM	2233	CD			412	57.550	54.426	3.003	1.00 51.73		C
MOTA	2234	NE			412	57.933	53.211	2.288	1.00 50.66		N
ATOM	2235	CZ			412	59.023	53.086	1.539	1.00 51.11		C
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MOTA	2236	NHl	ARG	Α	412	59.860	54.108	1.396	1.00	50.38	N
ATOM	2237		ARG			59.276	51.935	0.929	1.00	51.44	N
MOTA	2238	N	ALA			54.374	54.212	7.134	1.00		N
ATOM	2239	CA	ALA			54.321	53.057	8.031	1.00		C
		C	ALA			52.976	52.880	8.733	1.00		C
ATOM	2240										
ATOM	2241	0	ALA			52.495	51.757	8.877	1.00		0
MOTA	2242	CB	ALA			55.436	53.165	9.067	1.00		С
MOTA	2243	N	ARG			52.386	53.987	9.179	1.00	71.43	N
MOTA	2244	CA	ARG	Α	414	51.102	53.948	9.874	1.00	75.31	С
MOTA	2245	C	ARG	Α	414	49.999	53.373	8.991	1.00	77.02	С
ATOM	2246	0	ARG	Α	414	49.031	52.789	9.485	1.00	77.08	0
ATOM	2247	CB	ARG	A	414	50.683	55.353	10.322	1.00	76.52	С
ATOM	2248	CG	ARG	Α	414	51.456	55.939	11.491	1.00	78.03	C
ATOM	2249	CD	ARG	Α	414	50.703	57.153	12.026	1.00	80.11	С
ATOM	2250	NE			414	51.381	57.807	13.142	1.00		N
ATOM	2251	CZ			414	50.844	58.779	13.874	1.00		С
ATOM	2252		ARG			49.617	59.210	13.612	1.00		N
ATOM	2253		ARG				59.325	14.867	1.00		N
						51.532					
MOTA	2254 :				415	50.154	53.546	7.683	1.00		N
MOTA	2255	CA			415	49.170	53.058	6.725	1.00		C
MOTA	2256	С			415	49.252	51.540	6.520	1.00		С
MOTA	2257	0			415	49.489	51.069	5.403	1.00		0
MOTA	2258	CB	ASN	А	415	49.356	53.774	5.380	1.00	82.25	С
ATOM	2259	CG	ASN	A	415	48.070	53.845	4.568	1.00	83.78	С
ATOM	2260	OD1	ASN	A	415	47.434	52.825	4.295	1.00	84.64	0
MOTA	2261	ND2	ASN	A	415	47.681	55.055	4.181	1.00	84.44	N
MOTA	2262	N	TRP	Α	416	49.055	50.778	7.598	1.00	82.26	N
MOTA	2263	CA	TRP	Α	416	49.095	49.316	7.519	1.00	82.50	С
ATOM	2264	С			416	47.758	48.722	7.927	1.00		С
ATOM	2265	0			416	47.554	47.515	7.823	1.00		0
ATOM	2266	CB			416		48.732	8.412	1.00		C
ATOM	2267	CG			416	49.928	48.742	9.894	1.00		C
ATOM	2268		TRP			50.244	49.730	10.781	1.00		C
											C
ATOM	2269		TRP			49.273	47.714	10.659	1.00		
MOTA	2270		TRP			49.830	49.385	12.048	1.00		N
MOTA	2271		TRP			49.230	48.154	12.001	1.00		C
ATOM	2272	CE3			416	48.716	46.467	10.339	1.00		C
ATOM	2273		TRP			48.652	47.390	13.026	1.00		C
MOTA	2274	CZ3.	TRP	Α	416	 48.140	45.706	11.359	1.00	80.88	C
MOTA	2275	CH2	TRP	А	416	48.113	46.173	12.685	1.00	81.28	С
MOTA	2276	и	SER	Α	428	47.786	65.086	7.718	1.00	95.79	N
MOTA	2277	ĊA	SER	Α	428	48.357	66.353	7.278	1.00	95.93	С
ATOM	2278	C '	SER	Α	428	49.676	66.643	7.988	1.00	96.13	C
ATOM	2279	0	SER	А	428	50.268	67.709	7.812	1.00	96.06	0
ATOM	2280	CB			428	47.367	67.497	7.532	1.00	95.59	С
MOTA	2281	OG			428	47.047	67.610	8.907	1.00	95.03	0
MOTA	2282	N			429	50.134	65.687	8.789	1.00		N
ATOM	2283	CA			429	51.384	65.837	9.525	1.00		C
ATOM	2284	C			429	52.185	64.541	9.412	1.00		C
ATOM							63.685	8.586	1.00		0
	2285	O CP			429	51.867					C
ATOM	2286	CB			429	51.091	66.156	10.995	1.00		
ATOM	2287	CG			429	52.269	66.717	11.741	1.00		C
MOTA	2288		PHE			52.886	67.889	11.311	1.00		C
MOTA	2289		PHE			52.771	66.069	12.866	1.00		C
MOTA	2290		PHE			53.987	68.410	11.989	1.00		C
MOTA	2291	CE2	PHE	A	429	53.872	66.581	13.553	1.00	99.81	C
MOTA	2292	CZ	PHE	А	429	54.481	67.754	13.113	1.00	99.76	С

MOTA	2293	N	GLU	-		53.222	64.395	10.235	1.00	94.58			N
MOTA	2294	CA	GLU			54.047	.63.191	10.205	1.00	93.27			С
MOTA	2295	C	GLU	A	430	55.093	63.181	11.320	1.00	91.79			C
ATOM	2296	0	GLU	A	430	55.884	64.115	11.453	1.00	91.62			0
ATOM	2297	CB	GLU	A	430	54.728	63.065	8.841	1.00	94.00			C
ATOM .	2298	CG	GLU			55.300	61.691	8.559	1.00	94.70			C
ATOM	2299	CD	GLU			55.471	61.436	7.076		95.05			C
ATOM	2300		GLU			54.459	61.503	6.346		95.03			0
ATOM	2300		GLU			56.612	61.168	6.642		95.48			0
ATOM	2302	N Gr	GLU			55.092	62.110	12.110		89.87			N
ATOM	2303	CA	GLU			56.014	61.960	13.234		87.81			C
ATOM	2304	C	GLU			57.423	61.519	12.843		85.39			C
ATOM	2305	0	GLU	A	431	58.356	61.618	13.643	1.00	85.00			0
MOTA	2306	CB	GLU	Α	431 ⁻	55.437	60.973	14.257	1.00	89.03			C
ATOM	2307	CG	GLU	Α	431	54.235	61.494	15.044	1.00	90.63			C
MOTA	2308	CD	GLU	Α	431	53.091	61.955	14.153	1.00	91.93			C
MOTA	2309	OE1	GLU	Α	431	52.602	61.144	13.336	1.00	92.15			0
ATOM	2310	OE2	GLU			52.678	63.130	14.274	1.00	92.38			0
ATOM	2311	N	GLY			57.577	61.031	11.618		82.69			N
ATOM	2312	CA	GLY			58.885	60.587	11.170		79.01			C
ATOM		C				59.146	60.936			76.48			
	2313		GLY					9.720					C
ATOM	2314	0	GLY			58.345	61.623	9.087		76.66			0
ATOM	2315	N	VAL			60.269	60.464	9.190		73.56			N
MOTA	2316	CA	VAL			60.615	60.739	7.803		70.14			C
MOTA	2317	C	VAL	A	433	60.915	59.466	7.014		67.42			C
MOTA	2318	0	VAL	A	433	61.128	58.399	7.588	1.00	67.04	,		0
MOTA	2319	CB	VAL	Α	433	61.827	61.699	7.710	1.00	70.47			С
ATOM	2320	CG1	VAL	A	433	61.451	63.062	8.272	1.00	70.12			С
ATOM	2321	CG2	VAL	A	433	63.010	61.124	8.465		70.31			С
ATOM	2322	N	ASP			60.913	59.598	5.691		63.84			N
ATOM	2323	CA			434	61.173	58.491	4.778		60.33			C
ATOM	2324	C			434	62.386	58.864	3.930		58.07			C
ATOM	2325	0	ASP			62.300	59.737	3.066		57.72			0
ATOM	2326												C
		CB			434	59.937	58.261	3.899		60.27			
MOTA	2327	CG			434	60.115	57.123	2.914		60.71			C
ATOM	2328,		ASP			60.683	56.081	3.297		61.60			0
MOTA	2329		ASP			59.669	57.261	1.756		60.76			0
ATOM	2330	N .			435	63.516	58.207	4.181	1.00	55.22			N
ATOM	2331	CA			435	64.741	58.509	3.448	1.00	52.53			C
MOTA	2332	C	SER	Α	435	65.566	57.297	3.028	1.00	49.99			C
MOTA	2333	0	SER	Α	435	65.072	56.172	2.970	1.00	49.04			0
MOTA	2334	CB	SER	Α	435	65.620	59.437	4.284	1.00	53.18	,		С
MOTA	2335	OG	SER	A	435	65.947	58.820	5.515	1.00	54.44			0
ATOM	2336	N			436	66.838	57.550	2.740		47.61			N
MOTA	2337	CA			436	67.765	56.513	2.307		45.82			C
ATOM	2338	C			436	69.026	56.466	3.168		44.39			C
MOTA	2339	ō			436	69.481	57.490	3.685		44.28	1		0
ATOM	2340	CB			436	68.184	56.764			46.81			C
								0.858					
ATOM	2341	CG			436	67.075	56.643	-0.159		47.16			C
ATOM	2342		TYR			66.584	55.396	-0.537		47.36			C
ATOM	2343		TYR			66.527	57.778	-0.754		48.36		,	C
ATOM	2344		TYR			65.575	55.279	-1.485		49.05			C
ATOM	2,345	CE2	TYR			65.515	57.674	-1.706	1.00	49.53			C
ATOM	2346	CZ	TYR	А	436	65.046	56.422	-2.066		49.47			C
ATOM	2347	OH	TYR	A	436	64.050	56.312	-3.007	1.00	51.33			0
MOTA	2348	N	VAL	А	437	69.585	55.269	3.318	1.00	41.45			N
ATOM	2349	CA	VAL	A	437	70.817	55.089	4.072	1.00	38.90			C
								_					

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MOTA	2350	С	VAL	A	437	71.765	54.336	3.151	1.00 38.06	С
MOTA	2351	0	VAL	Α	437	71.334	53.496	2.366	1.00 37.46	0
MOTA	2352	CB	VAL	Α	437	70.600	54.275	5.370	1.00 38.21	C
ATOM	2353	CG1	VAL	A	437	69.639	55.014	6.286	1.00 38.54	C
ATOM	2354	CG2	VAL	Α	437	70.086	52.884	5.042	1.00 36.53	C
ATOM	2355	N	PRO			73.071	54.635	3.226	1.00 37.64	N
ATOM	2356	CA	PRO			74.049	53.958	2.371	1.00 36.86	С
		C	PRO			74.220	52.474	2.674	1.00 36.29	Ċ
ATOM	2357									
ATOM	2358	0	PRO			74.336	52.069	3.834	1.00 36.41	0
MOTA	2359	CB	PRO			75.327	54.764	2.608	1.00 36.76	C
ATOM	2360	CG	PRO			75.175	55.210	4.026	1.00 37.68	. C
ATOM	2361	CD	PRO			73.725	55.641	4.080	1.00 37.02	С
MOTA	2362	N	TYR	Α	439	74.223	51.671	1.613	1.00 35.21	N
MOTA	2363	CA	TYR	A	439	74.381	50.227	1.717	1.00 34.92	С
MOTA	2364	C	TYR	A	439	75.744	49.913	2.328	1.00 34.83	C
MOTA	2365	0	TYR	A	439	76.768	50.436	1.888	1.00 35.17	0
ATOM	2366	CB	TYR	Α	439	74.267	49.599	0.325	1.00 34.07	C
ATOM	2367	CG	TYR			74.418	48.098	0.299	1.00 33.14	С
ATOM	2368	CD1				73.561	47.279	1.029	1.00 32.78	C
ATOM	2369		TYR			75.407	47.494	-0.478	1.00 34.43	· c
							45.892	0.984	1.00 34.43	c
MOTA	2370		TYR			73.682				
MOTA	2371	CE2	TYR			75.536	46.110	-0.529	1.00 34.40	C
MOTA	2372	CZ	TYR			74.670	45.317	0.202	1.00 34.68	1 C
ATOM	2373	OH			439	74.791	43,949	0.148	1.00 36.73	0
ATOM	2374	N	ALA			75.752	49.051		1.00 34.57	N
MOTA	2375	CA	ALA	A	440	76.990	48.696	4.019	1.00 34.81	C
MOTA	2376	C	ALA	Α	440	77.361	47.225	3.860	1.00 34.72	, C
MOTA	2377	0	ALA	Α	440	78.375	46.776	4.390	1.00 34.93	. 0
MOTA	2378	CB	ALA	A	440	76.874	49.047	5.502	1.00 33.67	C
ATOM	2379	N	GLY	A	441	76.542	46.474	3.134	1.00 34.47	N
ATOM	2380	CA	GLY			76.833	45.066	2.945	1.00 34.40	С
MOTA	2381	C			441	76.172	44.203	4.003	1.00 34.97	С
MOTA	2382	0	GLY			75.144	44.581	4.567	1.00 35.10	0
ATOM	2383	N.			442	76.763	43.043	4.276	1.00 35.43	N
								5.265	1.00 35.43	C
ATOM	2384	CA			442	76.226	42.110			C
ATOM	2385	C			442	76.421	42.615	6.694	1.00 34.74	
ATOM	2386	0			442	77.415	43.272	7.005	1.00 33.81	0
ATOM	2387	CB			442	76.909	40.745	5.132	1.00 37.45	C
ATOM	2388	CG			442	76.860	40.138	3.739	1.00 41.47	C
ATOM	2389	CD.	LYS	Α	442	75.891	38.966	3.666	1.00 44.08	. C
MOTA	2390	CE	LYS	Α	442	74.461	39.409	3.914	1.00 47.03	С
MOTA	2391	NZ	LYS	Α	442	73.508	38.265	3.826	1.00 49.47	N
MOTA	2392	N	LEU	Α	443	75.466	42.282	7.555	1.00 33.84	N
ATOM	2393	CA	LEU	Α	443	75.497	42.663	8.962	1.00 33.05	С
ATOM	2394	С			443	76.769	42.197	9.681	1.00 33.87	C
MOTA	2395	0			443	77.401	42.968	10.398	1.00 32.69	0
ATOM	2396	CB			443	74.265	42.084	9.672	1.00 31.90	C
ATOM	2397	CG			443	74.104	42.252	11.190	1.00 31.99	c
	2398		LEU		-	72.651	42.031	11.568	1.00 31.10	C
MOTA			LEU					11.935	1.00 31.10	C
ATOM	2399					75.001	41.274			
ATOM	2400	N			444	77.135	40.934	9.481	1.00 34.24	N
ATOM	2401	CA			444	78.304	40.344	10.134	1.00 36.18	C
MOTA	2402	C			444	79.587	41.182	10.174	1.00 35.95	C
MOTA	2403	0			444	80.089	41.499	11.252	1.00 36.11	0
MOTA	2404	CB	LYS	A	444	78.621	38.981	9.510	1.00 37.74	C
MOTA	2405	CG	LYS	А	444	79.746	38.236	10.219	1.00 41.26	C
MOTA	2406	CD	LYS	A	444	79.871	36.804	9.720	1.00 44.01	C

MOTA	2407	CE	LYS	Α	444		80.857	36.013	10.560	1.00 44.57			С
ATOM	2408	NZ	LYS	Α	444		82.223	36.599	10.490	1.00 46.17			N
MOTA	2409	N	ASP	Α	445		80.113	41.530	9.005	1.00 35.90			N
MOTA	2410	CA	ASP	Α	445		81.347	42.301	8.904	1.00 36.42			С
MOTA	2411	C	ASP	Α	445		81.273	43.666	9.569	1.00 35.53			С
ATOM	2412		ASP				82.241	44.125	10.172	1.00 35.05			0
ATOM	2413	СВ	ASP				81.733	42.490	7.433	1.00 39.61			C
MOTA	2414	CG	ASP				81.951	41.172	6.713	1.00 42.27			С
ATOM	2415		ASP				82.810	40.383	7.163	1.00 43.65			0
ATOM	2416		ASP				81.262	40.927	5.700	1.00 45.22			0
ATOM	2417	N	ASN				80.126	44.317	9.447	1.00 34.05			N
ATOM	2418	CA	ASN					45.639	10.027	1.00 33.14			С
ATOM	2419	C	ASN				79.862	45.596	11.547	1.00 32.11			С
ATOM	2420	0	ASN				80.506	46.394	12.227.	1.00 31.82			0
	2421	CB	ASN				78.693	46.281	9.439	1.00 34.11			С
ATOM	2421	CG	ASN				78.853	46.608	7.969	1.00 35.94			С
ATOM	2422		ASN				79.391	47.659	7.612	1.00 37.15			0
ATOM			ASN				78.406	45.698	7.104	1.00 33.70			N
ATOM	2424				447		79.071	44.669	12.078	1.00 31.18			N
ATOM	2425	N					78.929	44.533	13.523	1.00 30.87			C
MOTA	2426	CA			447		80.273	44.161	14.154	1.00 31.57			Ċ
MOTA	2427	C	VAL				_	44.101	15.233	1.00 31.53			0
MOTA	2428	0	VAL				80.621		13.882	1.00 30.26			C
MOTA	2429	CB			447		77.883	43.454	15.354	1.00 30.20			C
MOTA	2430		VAL				77.995	43.087		1.00 29.78			C
MOTA	2431		VAL				76.490	43.969	13.581	1.00 23.00			N
ATOM	2432	N			448		81.030	43.313	13.468				C
ATOM	2433	CA			448		82.326	42.887	13.971	1.00 33.06			C
MOTA	2434	C			448		83.279	44.082	14.049	1.00 31.22			0
MOTA	2435	0			448		83.975	44.257	15.042	1.00 29.89			
MOTA	2436	CB			448		82.900	41.790	13.066	1.00 35.76			. C
ATOM	2437	CG			448		84.250	41.240	13.503	1.00 41.89			C
MOTA	2438	CD			448		84.719	40.085	12.623	1.00 46.86			C
MOTA	2439	OE1	GLU				84.030	39.037	12.596	1.00 49.61			0
MOTA	2440	OE2			448		85.770	40.228	11.957	1.00 47.95			0
MOTA	2441	N			449	•	83.302	44.904	13.004	1.00 29.89			N
MOTA	2442	CA	ALA	Α	449		84.167	46.083	12.982	1.00 29.27			C
MOTA	2443	C			449		83.764	47.074	14.075	1.00 28.76			C
MOTA	2444	Ο.	ALA	A	449		84.619	47.677	14.725	1.00 28.88			0
MOTA	2445	CB	ALA	Α	449		84.099	46.764	11.616	1.00 28.30			C
MOTA	2446	N	SER	Α	450				14.267	1.00 27.76			N
MOTA	2447	· CA			450		81.947	48.157	15.282	1.00 27.63			C
ATOM	2448	C	SER	A	450		82.321	47.712	16.691	1.00 27.22			C
ATOM	2449	0	SER	Α	450		82.815	48.507	17.490	1.00 26.61			0
ATOM	2450	CB	SER	A	450		80.421	48.272	15.182	1.00 27.03			С
ATOM	2451	OG	SER	A	450		80.037	49.038	14.053	1.00 28.56			0
ATOM	2452	N	LEU	Α	451		82.086	46.437	16.989	1.00 26.98			N
MOTA	2453	CA	LEU	Α	451		82.378	45.906	18.310	1.00 27.66			C
ATOM	2454	С	LEU	Α	451		83.870	45.755	18.598	1.00 29.12			C
MOTA	2455	0	LEU	Α	451		84.270	45.719	19.758	1.00 28.46			0
MOTA	2456	CB	LEU	Α	451		81.638	44.580	18.522	1.00 26.68			C
ATOM	2457	CG	LEU	Α	451		80.112	44.754	18.493	1.00 26.86			С
MOTA	2458				451		79.422	43.455	18.852	1.00 24.50			C
ATOM	2459				451		79.704	45.860	19.461	1.00 26.58		1	C
ATOM	2460	N			452		84.697	45.671	17.559	1.00 30.10			N
ATOM	2461	CA			452		86.132	45.577	17.795	1.00 31.68			С
ATOM	2462	C			452		86.595		18.323	1.00 31.06			С
ATOM	2463	Ö			452		87.470	46.999	19.187				0
		_											

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MOTA	2464	CB	ASN	A	452	86.907	45.230	16.519	1.00 33.39		C
ATOM	2465	CG	ASN	А	452	86.881	43.747	16.208	1.00 37.58		С
MOTA	2466	OD1	ASN	A	452	86.800	42.908	17.113	1.00 40.20		0
MOTA	2467	ND2	ASN	A	452	86.969	43.411	14.925	1.00 39.30		N
MOTA	2468	N	LYS	A	453	86.000	47.996	17.805	1.00 30.67		N
ATOM	2469	CA	LYS	А	453	86.358	49.334	18,256	1.00 31.02		С
ATOM	2470	C	LYS			85.863	49.550	19.680	1.00 28.53		С
MOTA	2471	0	LYS			86.549		20.489	1.00 28.63		0
MOTA	2472	CB	LYS			85.779	50.407	17.326	1.00 32.56		С
ATOM	2473	CG	LYS			86.475	50.454	15.974	1.00 38.18		С
ATOM	2474	CD	LYS			86.326	51.813	15.290	1.00 40.85		C
ATOM	2475	CE	LYS			84.888	52.108	14.928	1.00 43.86		C
ATOM	2476	NZ	LYS			84.745	53.424	14.236	1.00 45.10		N
MOTA	2477	N	VAL			84.674	49.041	19.982	1.00 26.35		N
ATOM	2478	CA			454	84.121	49.168	21.321	1.00 25.14		C
ATOM	2479	C	VAL			85.037	48.436	22.305	1.00 25.64		Ċ
ATOM	2480	0			454	85.395	48.980	23.352	1.00 24.53		Ó
MOTA	2481	CB				82.700	48.566	21.409	1.00 25.38		C
ATOM	2482		VAL			82.241	48.504	22.869	1.00 24.56		c
ATOM	2483		VAL			81.725	49.413	20.589	1.00 24.60		Ċ
ATOM	2484	N			455	85.419	47.208	21.956	1.00 25.47	*	N
ATOM	2485	CA			455	86.290	46.393	22.805	1.00 26.49		C
MOTA	2486	C			455	87.634	47.073	23.053	1.00 27.06		Ċ
ATOM	2487	Ō			455	88.162	47.051	24.165	1.00 26.76		o
ATOM	2488	CB			455	86.534	45.030	22.157	1.00 26.81		Č
ATOM	2489	CG			455	85.335	44.099	22.139	1.00 27.88		C
MOTA	2490	CD			455	85.653	42.889	21.279	1.00 29.25		C
ATOM .	2491	CE			455	84.558	41.857	21.344	1.00 32.72		C
MOTA	2492	NZ			455	84.871	40.695	20.464	1.00 33.72		N
ATOM	2493	N			456	88.185	47.664	22.000	1.00 26.88		N
ATOM	2494	CA			456	89.463	48.355	22.084	1.00 28.22		C
MOTA	2495	C			456	89.356	49.563	23.021	1.00 27.71		C
MOTA	2496	0			456	90.221	49.788	23.868	1.00 27.71		o
ATOM	2497	CB			456	89.896	48.801	20.684	1.00 29.36		С
ATOM	2498	OG			456	91.173	49.401	20.715	1.00 32.57		0
ATOM	2499	N			457	88.289	50.339	22.866	1.00 26.02		N
ATOM	2500	CA			457	88.083	51.502	23.713	1.00 25.29		C
ATOM	2501	C			457	87.905	51.052	25.159	1.00 24.88		C
ATOM	2502	0			457	88.407	51.692	26.083	1.00 25.60		0
ATOM	2502	CB			457	86.847	52.297	23.269	1.00 24.46		C
ATOM	2504		THR			87.013	52.689	21.904	1.00 26.98		o
ATOM	2505	CG2				86.677	53.541	24.113	1.00 21.68	,	· C
ATOM	2506	N			458	87.192	49.948	25.355	1.00 24.86		N
ATOM	2507	CA			458	86.977	49.430	26.697	1.00 23.62		C
ATOM	2508	C			458	88.314	49.140	27.363	1.00 24.86		C
MOTA	2509	0			458	88.496	49.424	28.545	1.00 25.51		0
MOTA	2510	CB			458	86.097	48.179	26.653	1.00 23.91		C
ATOM	2511	CG			458	84.603	48.501	26.525	1.00 23.56		C
ATOM	2512	SD			458	83.557	47.082	26.176	1.00 24.90		s
ATOM	2513	CE			458	83.569	46.235	27.743	1.00 23.81		C
MOTA	2514	N			459	89.268	48.599	26.613	1.00 25.01		И
MOTA	2515	CA			459	90.567	48.321	27.213	1.00 20.31		C
MOTA	2516	C			459	91.294	49.613	27.561	1.00 27.49		C
ATOM	2517	0			459	92.055	49.655	28.528	1.00 27.52		0
ATOM	2518	СВ			459	91.418	47.440	26.300	1.00 27.32		C
MOTA	2519	SG			459	90.985	45.676	26.452	1.00 23.11		s
ATOM	2520	N			460	91.052	50.665	26.780	1.00 26.76		N
	~220		* 1014	47	100	J2.0J2	50.005	20.,00	2.00 20.70		

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ATOM	2521	CA	ASN	Α	460	91.659	51.966	27.053	1.00 26.30		С
MOTA	2522	C	ASN	А	460	91.112	52.452	28.387	1.00 25.18		С
ATOM	2523	0	ASN	·A	460	91.780	53.177	29.110	1.00 25.85		0
ATOM	2524	CB	ASN	Α	460	91.284	52.996	25.983	1.00 26.49		С
MOTA	2525	CG	ASN	Α	460	91.974	52.753	24.662	1.00 27.93		С
ATOM	2526		ASN			91.321	52.628	23.629	1.00 30.37		0
ATOM	2527		ASN			93.301	52.698	24.683	1.00 27.47		N
ATOM	2528	N	CYS			89.886	52.049	28.704	1.00 24.75		N
	2529	CA ·	CYS				52.468		1.00 24.75		C
ATOM						89.245		29.946			
ATOM	2530	C	CYS			89.471	51.485	31.093	1.00 24.59		C
MOTA	2531	0	CYS			88.929	51.663	32.179	1.00 24.19		0
ATOM	2532	CB	CYS			87.738	52.665	29.716	1.00 25.37		C
MOTA	2533	SG	CYS	•		87.342	53.931	28.465	1.00 26.44		S
MOTA	2534	N	GLY			90.266	50.449	30.839	1.00 25.17		N
ATOM	2535	CA	GLY	A	462	90.562	49.454	31.857	1.00 24.26		C
MOTA	2536	C	GLY			89.424	48.490	32.136	1.00 25.01		C
ATOM	2537	0	GLY	Α	462	89.300	47.970	33.250	1.00 25.14		Ō
MOTA	2538	N	ALA	A	463	88.601	48.228	31.127	1.00 23.44		N
MOTA	2539	CA	ALA	Α	463	87.462	47:339	31.302	1.00 23.93		С
ATOM	2540	C	ALA	A	463	87.479	46.110	30.397	1.00 24.29		С
MOTA	2541	0	ALA			87.688	46.216	29.185	1.00 23.39		0
ATOM	2542	CB	ALA			86.169	48.122	31.085	1.00 21.46		С
ATOM	2543	N	LEU			87.245	44.950	31.002	1.00 24.49		N
ATOM	2544	CA	LEU			87.195	43.686	30.275	1.00 26.40		C
ATOM	2545	C	LEU			85.749	43.260	30.066	1.00 25.77		C
ATOM	2546	0	LEU			85.476	42.351	29.287	1.00 27.45		0
ATOM	2547	CB	LEU			87.936	42.582	31.039	1.00 27.15		C
MOTA	2548	CG	LEU			89.448	42.499	30.823	1.00 27.05		C
ATOM			LEU			90.024			1.00 29.00		C
	2549						41.335	31.630	1.00 31.00		C
ATOM	2550	CD2				89.730	42.304	29.349			
ATOM	2551	N			465	84.829	43.909	30.775	1.00 25.23		N
MOTA	2552	CA			465	83.406	43.603	30.656	1.00 24.98		C
MOTA	2553	C			465	82.589	44.893	30.684	1.00 25.79		C
ATOM	2554	0			465	83.096	45.955	31.057	1.00 24.88		0
MOTA	2555	CB	THR			82.913	42.719	31.812	1.00 25.00		С
ATOM	2556	OG1	THR			82.998	43.458	33.035	1.00 24.92		0
MOTA	2557	CG2	THR	Α	465	83.757	41.447	31.921	1.00 24.20		С
MOTA	2558	N	ILE	Α	466	81.323	44.801	30.293	1.00 24.73		N
ATOM.	2559	CA	ILE,	Α	466	80.470	45.977	30.294	1.00 24.59	* . * .	C
MOTA	2560	Ċ	ILE	A	466	80.269	46.503′	31.717	1:00 24.91		C
ATOM	2561	0	ILE	А	466	80.359	47.702	31.952	1.00 26.03		0
MOTA	2562	CB	ILE	Α	466	79.117	45.672	29.616	1.00 24.22		С
ATOM	2563	CG1	ILE	Α	466	79.340	45.548	28.104	1.00 22.81		С
MOTA	2564	CG2	ILE	Α	466	78.095	46.761	29.931	1.00 20.91		С
MOTA	2565	CD1	ILE	Α	466	78.132	45.051	27.344	1.00 23.02		·C
ATOM	2566	N			467	79.997	45.614	32.688	1.00 25.66		N
MOTA	2567	CA	PRO			79.811	46.107	34.058	1.00 25.52		С
MOTA	2568	C			467	81.057	46.840	34.566	1.00 26.38		C
ATOM	2569	Ō			467	80.967	47.837	35.284	1.00 25.66		ō
ATOM	2570	CB			467	79.525	44.829	34.846	1.00 25.82		C
ATOM	2571	CG			467	78.798	43.980	33.829	1.00 25.02		C
ATOM	2572	CD			467	79.658	44.181	32.596	1.00 23.13		C
-									1.00 24.50	•	
ATOM	2573	N	GLN			82.225	46.346	34.183			N
MOTA	2574	CA	GLN			83.464	46.968	34.609	1.00 27.70	•	C
ATOM	2575	C.	GLN			83.626	48.344	33.954	1.00 28.31		C
ATOM	2576	0	GLN			84.153	49.279	34.567	1.00 27.56		0
MOTA	2577	CB	GLN	A	468	84.631	46.052	34.265	1.00 29.61		С

MOTA	2578	CG	GLN	Α	468	85.932	46.460	34.882	1.00 32.72		C
MOTA	2579	CD	GLN			86.925	45.320	34.922	1.00 32.87		C
MOTA	2580	OE1	GLN	A	468	87.034	44.540	33.977	1.00 30.31		0
MOTA	2581	NE2	GLN			87.670	45.231	36.015	1.00 35.10		N
ATOM	2582	N	LEU			83.156	48.468	32.713	1.00 27.10		N
ATOM	2583	CA	LEU			83.222	49.734	31.994	1.00 26.38		C
MOTA	2584	C	LEU			82.286	50.742	32.656	1.00 25.76		С
ATOM	2585	0	LEU			82.641	51.904	32.840	1.00 24.62		0
MOTA	2586	CB	LEU			82.809	49.547	30.530	1.00 26.12		С
ATOM	2587	CG	LEU			82.606	50.848	29.742	1.00 26.70		C
ATOM	2588	CD1				83.947	51.530	29.499	1.00 24.80		C
MOTA	2589		LEU			81.920	50.538	28.421	1.00 26.30		С
ATOM	2590	N	GLN			81.092	50.285	33.018	1.00 24.81		N
ATOM	2591	CA	GLN			80.101	51.148	33.652	1.00 26.06		C.
MOTA	2592	C			470	80.595	51.643	35.004	1.00 27.46		C
ATOM	2593	0	GLN			80.229	52.723	35.473	1.00 27.35		Ó
ATOM	2594	CB	GLN			78.779	50.383	33.798	1.00 25.66		C
MOTA	2595.	CG	GLN			78.145	50.108	32.437	1.00 26.19		C
MOTA	2596	CD	GLN			76.907	49.240	32.484	1.00 27.08	₹	C
ATOM	2597	OE1				76.089	49.270	31.561	1.00 28.25		0
ATOM	2598	NE2	GLN			76.768	48.452	33.537	1.00 24.83		N
ATOM	2599	N			471	81.464	50.855	35.611	1.00 27.91		N
MOTA	2600	CA			471	82.008	51.194	36.909	1.00 29.16		C
MOTA	2601	C ·	SER			83.245	52.094	36.831	1.00 28.62		C
ATOM	2602	0			471	83.387	53.028	37.618	1.00 29.46		0
ATOM	2603	CB			471	82.346	49.901	37.660	1.00 28.43		C
MOTA	2604	OG N			471	82.917	50.183	38.920 35.863	1.00 33.24 1.00 28.60	•	N
ATOM ATOM	2605 2606	N CA	LYS		472	84.116	51.832 52.578	35.732	1.00 28.80		C
ATOM	2607	CA	LYS			85.368 85.459	53.725	34.728	1.00 28.32		C
ATOM	2607	0	LYS			86.386	54.526	34.728	1.00 27.30		0
ATOM	2609	CB	LYS			86.499	51.591	35.437	1.00 28.80		C
ATOM	2610	CG	LYS			86.598	50.469	36.445	1.00 20.00		C
ATOM	2611	CD	LYS			87.547	49.371	35.990	1.00 32.26	•	C
ATOM	2612	CE	LYS			88.992	49.826	35.994	1.00 33.68	•	C
MOTA	2613	NZ			472	89.910	48.692	35.671	1.00 34.81		N
ATOM	2614	N	ALA			84.523	53.811	33.789	1.00 26.86		N
ATOM	2615	CA			473	84.586	54.866	32.784	1.00 26.51		C
ATOM	2616	C			473	84.672	56.284	33.351	1.00 26.27		
ATOM	2617	0			473	83.986	56.637	34.313	1.00 26.64	•	0
MOTA	2618	CB	ALA			83.394	54.760	31.831	1.00 26.47		C
ATOM	2619	N			474	85.544	57.080	32.742	1.00 25.53		N
MOTA	2620	CA			474	85.746	58.476	33.110	1.00 25.18		C
MOTA .	2621	С	LYS	Α	474	85.178	59.222	31.911	1.00 25.48		С
MOTA	2622	0	LYS	Α	474	85.742	59.190	30.816	1.00 25.05		0
ATOM	2623	CB	LYS	А	474	87.237	58.749	33.293	1.00 23.52		С
MOTA	2624	CG	LYS	Α	474	87.842	57.916	34.425	1.00 25.87		С
MOTA	2625	CD	LYS	Α	474	89.333	57.657	34.217	1.00 24.85		С
ATOM	2626	CE	LYS	A	474	90.152	58.924	34.356	1.00 25.06		С
MOTA	2627	NZ	LYS	A	474	91.582	58.631	34.061	1.00 25.87		N
MOTA	2628	N	ILE	A	475	84.044	59.881	32.118	1.00 25.73		N
MOTA	2629	CA			475	83.361	60.558	31.025	1.00 25.74		С
MOTA	2630	C			475	83.328	62.069	31.166	1.00 25.52		C
MOTA	2631	0			475	82.858	62.598	32.173	1.00 25.22		0
MOTA	2632	CB			475	81.912	60.020	30.906	1.00 26.10		C
MOTA	2633		ILE			81.934	58.482	30.888	1.00 25.99		С
MOTA	2634	CG2	ILE	A	475	81.254	60.550	29.639	1.00 27.00		C

MOTA	2635	CD1	ILE	A	475	80.559	57.819	30.973	1.00 22.84	C
MOTA	2636	N	THR	A	476	83.833	62.766	30.154	1.00 25.28	N
MOTA	2637	CA	THR	A	476	83.839	64.220	30.199	1.00 24.69	C
MOTA	2638	C	THR	Α	476	82.968	64.853	29.137	1.00 24.58	C
ATOM	2639	0	THR	A	476	82.822	64.340	28.026	1.00 23.13	0
MOTA	2640	CB	THR	Α	476	85.254	64.819	30.029	1.00 24.42	C
MOTA	2641	OG1	THR			85.179	66.245	30.177	1.00 24.64	0
MOTA	2642	CG2	THR			85.817	64.506	28.641	1.00 21.62	С
ATOM	2643	N	LEU			82.392	65.985	29.504	1.00 25.11	N
ATOM	2644	CA			477	81.568	66.751	28.599	1.00 26.78	C
ATOM	2645	C	LEU			82.580	67.571	27.798	1.00 26.72	C
ATOM	2646	0	LEU			83.672	67.855	28.290	1.00 26.01	ō
ATOM	2647	CB			477	80.645	67.668	29.405	1.00 27.13	C
ATOM	2648	CG			477	79.566	68.443	28.661	1.00 28.34	C
ATOM	2649		LEU			78.598	67.476	27.985	1.00 27.41	C
ATOM	2650	CD2				78.838	69.331	29.653	1.00 27.41	C
							67.924	•	1.00 27.82	N
ATOM	2651	N			478	82.221		26.569		C
ATOM	2652	CA	VAL			83.075	68.708	25.678	1.00 28.66 1.00 29.15	
ATOM	2653	C	VAL			82.407	70.062	25.415		C
	.2654	0	VAL			81.186	70.143	25.327	1.00 28.79	0
ATOM	2655	CB			478	83.275	67.964	24.342	1.00 30.20	C
ATOM	2656	CG1				83.918	68.870	23.326	1.00 33.41	C
MOTA	2657	CG2	VAL			84.133	66.731	24.563	1.00 30.57	C
MOTA	2658	N			479	83.200	71.121	25.288	1.00 29.64	N
MOTA	2659	CA			479	82.645	72.455	25.054	1.00 31.24	С
MOTA	2660	С	SER	Α	479	82.016	72.595	23.675	1.00 32.88	С
MOTA	2661	0	SER	Α	479	82.376	71.878	22.745	1.00 32.90	0
MOTA	2662	CB	SER	Α	479	83.731	73.523	25.208	1.00 28.66	C
MOTA	2663	OG	SER	Α	479	84.669	73.432	24.151	1.00 29.51	0
MOTA	2664	N	SER	Α	480	81.075	73.528	23.556	1.00 36.21	N
ATOM	2665	CA	SER	Α	480	80.389	73.798	22.290	1.00 40.17	C
ATOM	2666	C	SER	Α	480	81.393	74.060	21.172	1.00 41.93	C
ATOM	2667	0	SER	Α	480	81.303	73.479	20.091	1.00 42.38	0
ATOM	2668	CB	SER	Α	480	79.487	75.026	22.429	1.00 40.09	C
MOTA	2669	OG			480	78.558	74.864	23.482	1.00 42.83	0
ATOM	2670	N			481	82.346	74.948	21.447	1.00 44.79	N
ATOM	2671	CA			481	83.377	75.316	20.483	1.00 47.03	С
MOTA	2672	С	VAL	Α	481	84.169	74.125	19.958	1.00 48.55	С
MOTA	2673	0			481	84.514	. 74.083	18.778	1.00 49.15	0
ATOM	2674	CB			481	84.368	76.327	21.091	1.00 46.95	C
MOTA	2675		VAL			85.504	76.593	20.111	1.00 47.91	C
ATOM	2676		VAL			83.646	77.625	21.420	1.00 47.48	C
ATOM	2677	N			482	84.466	73.168		1.00 50.46	N
ATOM	2678	CA			482	85.219	71.982	20.438	1.00 52.74	C
ATOM	2679	C			482	84.505	71.250	19.312	1.00 54.09	C
ATOM	2680	0			482	85.131	70.520	18.543	1.00 54.30	0
ATOM	2681	CB			482	85.381	71.022	21.620	1.00 54.30	C
ATOM	2682					86.013	71.650		1.00 52.72	
		OG N			482			22.718		0
ATOM	2683	N CA			483	83.193	71.446	19.222	1.00 55.12	N
ATOM	2684	CA			483	82.391	70.791	18.194	1.00 56.51	C
ATOM	2685	C			483	82.101	71.737	17.026	1.00 56.96	C
ATOM	2686	0			483	82.516	71.404	15.895	1.00 58.03	0
ATOM	2687	CB			483	81.063	70.276	18.792	1.00 56.37	C
ATOM	2688		ILE			81.355	69.431	20.037	1.00 56.23	C
ATOM	2689		ILE			80.304	69.450	17.763	1.00 56.35	C
ATOM	2690	CD1	ILE			80.121	69.014	20.813	1.00 56.41	С
TER	2691		ILE	A	483					

HETATM	2692	K	K	Α	900	94.574	53.191	29.387	0.75	33.20		K
HETATM	2693	P	XMP		602	68.081	55.369	14.890	1.00	29.26		Þ
HETATM	2694	01P	XMP		602	67.684	55.295	13.481	1.00	30.18		0
HETATM	2695	02P	XMP		602	68.902	54.234	15.354	1.00	31.70		0
HETATM	2696	05'	XMP		602	66.787	55.392	15.717	1.00	28.83		0
HETATM	2697	03P	XMP		602 -	68.651	56.672	15.275	1.00	30.39		0
HETATM	2698	C5 '	XMP		602	65.796	54.347	15.863	1.00	26.57		С
HETATM		C4 '	XMP		602	64.756	54.593	16.960		26.90		С
HETATM		04 '	XMP		602	63.943	55.732	16.688		27.02		0
HETATM		C1'	XMP		602	62.618	55.681	17.180		27.81		Ċ
HETATM		N9	XMP		602	61.690	55.953	16.031		28.12		N
HETATM		C4	XMP		602	61.248	57.183	15.601		28.78		C
HETATM		N3	XMP		602	61.556	58.444	16.121		29.01		N
HETATM		N1	XMP		602	60.086	59.258	14.353		29.05		N
HETATM		C2	XMP		602	60.942	59.481	15.459		30.77		C
HETATM		02	XMP		602	61.128	60.639	15.829		31.42		0
HETATM		C6	XMP		602	59.764	57.989	13.823		27.88		C
HETATM		06	XMP		602	59.015	57.875	12.853		28.97		0
HETATM		C5	XMP		602	60.406	56.909	14.506		28.31		C
HETATM		N7	XMP		602	60.325	55.573	14.268		27.77		N
												C
HETATM		C8	XMP		602	61.076	55.082	.15.166		27.54		
HETATM		C2 '	XMP		602	62.604	54.298	17.878		26.62		С
HETATM		02'	XMP		602	62.808	54.554	19.261		26.73		0
HETATM		C3 '	XMP		602	63.705	53.537	17.141		26.75		C
HETATM		03 '	XMP		602	64.161	52.438	17.926		26.88		0
HETATM		C1	AOM		600	60.161	58.910	19.598		39.69		C
HETATM		C2	AOM		600	55.659	56.950	16.499		41.87		C
HETATM		C3	MOA		600	54.526	56.264	16.209		42.80		C
HETATM		C4	AOM		600	53.214	56.947	16.563		43.33		C
HETATM		C5	AOM		600	52.615	56.311	17.824		44.46		С
HETATM		C6	AOM		600	53.260	56.803	19.110		45.19		С
HETATM		C7	MOA		600	59.586	54.022	20.007		38.55		С
HETATM		C8	MOA		600	56.536	53.702	18.367		39.77		С
HETATM		C9	AOM		600	54.498	54.877	15.549		42.56		С
HETATM		C10	AOM		600	60.713	56.925	20.765		38.97		С
HETATM		C11	MOA		600	59.765	56.576	19.638	1.00	38.97		C
HETATM	2728		MOA		600	59.227	55.285	19.257		38.94		С
HETATM	2729	C13	AOM		600	58.328	55.252	18.116	1.00	38.60		С
HETATM	2730		MOA		600	58.002	56.474	17.412	1.00	39.76		C
HETATM	2731	C15	AOM		600	58.558	57.736	17.831		39.72		C
HETATM	2732.		MOA		600 .	59.443	57.754		1.00	39.74		С
HETATM	2733	C17	AOM		600	57.066	56.441	16.206	1.00	41.19		C
HETATM	2734	01	AOM		600	60.164	60.070	19.326	1.00	40.10		0
HETATM		02	MOA		600	60.857	58.377	20.607	1.00	39.52		0
HETATM	2736	03	MOA		600	57.806	54.039	17.729	1.00	38.84		0
HETATM	2737	04	MOA		600	58.226	58.894	17.131	1.00	41.40		0
HETATM	2738	05	MOA		600	53.221	58.031	19.364	1.00	46.62		0
HETATM	2739	06	MOA		600	53.815	55.961	19.854	1.00	44.12		0
MTATAH	2740	0	HOH		1	61.376	37.927	37,348	1.00	48.46		0
HETATM	2741	0	HOH		2	66.118	60.676	24.768	.1.00	20.39		0
HETATM	2742	0	нон		3	57.906	58.970	28.360	1.00	26.84		0
HETATM	2743	0	HOH		4 .	66.772	48.007	38.757	1.00	25.49		0
HETATM	2744	0	HOH		5	87.612	55.755	31.226	1.00	23.33		0
HETATM	2745	0	HOH		6	79.992	42.156	29.537		21.25		0
HETATM		0	нон		7	59.636	45.401	36.922	1.00	29.33		0
HETATM		0	нон		8	71.079	54.650	21.993		25.95		0
HETATM	2748	0	HOH		9	75.154	45.933	32.815		29.51		0

HETATM	2749	0	HOH	10	84.715	43.023	9.513	1.00 52.28		0
HETATM	2750	0	HOH	11	78.040	54.255	34.365	1.00 26.73		0
HETATM	2751	0	HOH	12	56.541	77.341	37.146	1.00 29.92		0
HETATM	2752	0	HOH	13	71.260	53.575	14.099	1.00 27.29		0
HETATM	2753	0	HOH	14	76.501	44.082	31.079	1.00 23.02		0
HETATM	2754	0	HOH	15	56.998	79.001	34.463	1.00 24.15		0
HETATM	2755	0	нон	16	73.891	57.573	36.189	1.00 25.33		0
HETATM	2756	0	HOH	17	79.049	48.291	37.245	1.00 34.20		0
HETATM		0	нон	18	84.628	53.459	21.080	1.00 24.55		0
HETATM		0	нон	19	60.274	50.551	20.190	1.00 29.66		0
HETATM	2759	0	нон	20	88.720	54.039	33.349	1.00 25.23		0
HETATM	2760	0	нон	21	72.841	38.348	33.765	1.00 30.16		0
HETATM		0	нон	22	66.292	58.791	21.349	1.00 29.06		0
HETATM	2762	0	нон	23	67.212	67.480	30.959	1.00 23.37		0
HETATM		0	НОН	24	64.926	73.569	32.978	1.00 27.92		0
HETATM		Ō	НОН	25	74.543	60.063	37.886	1.00 37.97	•	0
HETATM		0	НОН	26	70.536	33.662	27.436	1.00 32.78		0
HETATM		0	нон	27	49.672	44.473	20.960	1.00 32.61		0
HETATM		Ō	НОН	28	82.525	67.407	31.912	1.00 36.84		0
HETATM		Ō	нон	29	62.576	38.739	33.869	1.00 27.93		0
HETATM		ō	НОН	. 30	65.657	36.916	34.650	1.00 31.90		Ō
HETATM		0	НОН	31	77.268	36.846	6.578	1.00 54.28		0
HETATM		ō	нон	. 32	53.069	53.133	19.199	1.00 50.49	•	0
HETATM		Ö	нон	33	76.732	41.427	32.285	1.00 26.63		ō
HETATM		.0	нон	34	59.082	42.334	5.797	1.00 52.93		o
HETATM		Ö	нон	35	75.506	39.010	8.246	1.00 30.82		0
HETATM		Ö	нон	36	69.343	68.054	32.924	1.00 32.47		0
HETATM		Ö	нон	37	64.457	56.749	20.210	1.00 32.67		Ö
HETATM		0	нон	38	62.747	61.776	37.438	1.00 35.12		Ö
HETATM		Ö	нон	39	73.816	64.979	30.707	1.00 34.05		o
HETATM		0	нон	40	64.885	41.594	7.798	1.00 31.03		ŏ
HETATM		.0	нон	41	87.291	69.760	24.178	1.00 33.68		o
HETATM		0	нон	42	63.521	39.537	6.109	1.00 44.37		0
HETATM		0	нон	43	65.271	63.920	35.809	1.00 34.06		o
HETATM		0	нон	44	56.965	57.545	38.806	1.00 37.58		0
HETATM		0	нон	45	79.547	40.499	32.022	1.00 37.32		0
HETATM		0	нон	46	60.019	51.355	9.831	1.00 30.80		0
HETATM		0	нон	47	61.960	50.701	17.845	1.00 28.12		0
HETATM		0	нон	48	74.307	50.935	36.302	1.00 32.12		o
HETATM		0	нон	49	48.640	54.380	36.947	1.00 32.12		0
HETATM		0	нон	50	53.284	51.835	37.998	1.00 35.47		o
HETATM		0	нон	51	51.464	58.781	25.814	1.00 42.15		0
HETATM		0	нон	52	66.312	31.378	26.604	1.00 42.30		0
HETATM		0	нон	53	51.114	46.450	35.768	1.00 39.78		0
HETATM		Ö	НОН	54	72.161	53.847	44.046	1.00 49.25		0
HETATM		0	нон	55	68.174	38.435	46.467	1.00 39.10	,	0
HETATM		0	НОН	56	62.329	64.325	35.245	1.00 33.10		0
HETATM		0	нон	57	56.533	41.432	37.289	1.00 31.02		0
HETATM		o	нон	58	60.631	39.846	6.689	1.00 42.73		0
HETATM		0	нон	59	54.566	73.818	39.035	1.00 42.47	•	0
HETATM		0	нон	60	60.006	59.911	30.562	1.00 39.12		0
HETATM		0	нон	61	93.037	49.413	23.367	1.00 39.12		0
HETATM		0	НОН	62	78.413	51.159	38.006	1.00 33.30		0
HETATM		0	нон	63	66.743	37.946	16.658	1.00 31.22		0
HETATM		0	нон	64	61.454	73.868	39.323	1.00 31.22		0
HETATM		0	нон	65	52.424	53.998	25.927	1.00 45.74		0
HETATM		0	HOH	66	59.056	45.472	5.839	1.00 30.17		0
	2000	9	11011	55	55.050	43.472	5.055	1.00 44.00		J

HETATM	2806	0	нон	67	71.714	56.136	41.913	1.00 33.23 。	0
HETATM	2807	0	HOH	68	92.961	54.326	36.232	1.00 47.69	0
HETATM	2808	0	HOH	69	82.193	63.483	21.263	1.00 31.53	· O
HETATM	2809	0	HOH	70	80.771	49.496	10.878	1.00 59.85	0
HETATM	2810	0	HOH	71	50.884	32.054	16.328	1.00 46.83	0
HETATM	2811	0	HOH	. 72	43.572	44.049	23.478	1.00 40.54	- 0
HETATM	2812	0	HOH	73	79.532	38.613	17.574	1.00 40.24	0
HETATM	2813	0	HOH	74	94.403	49.046	26.001	1.00 45.47	0
HETATM	2814	0	HOH	75	59.694	51.808	16.401	1.00 31.05	0
HETATM		0	нон	76	72.250	67.511	32.157		0
HETATM	2816	0	HOH	77	62.657	53.868	-3.472	1.00 54.27	
HETATM		0	HOH	78	51.622	50.791	21.993	1.00 42.86	0
HETATM		0	HOH	79	92.002	50.835	35.387	1.00 48.05	0
HETATM		0	нон	80	59.267	38.498	34.638	1.00 33.40	0
HETATM		0	нон	81	90.144	53.498	35.941	1.00 39.87	0
HETATM		0	нон	82	78.700	70.970	25.462	1.00 45.50	0
HETATM		0	нон	83	75.528	70.617	31.893	1.00 36.82	0
HETATM		0	нон	84	58.864	51.527	22.923	1.00 41.16	0
HETATM		0	нон	85	85.509	49.375	39.516	1.00 46.27	0
HETATM		Ö	нон	86	75.401	39.056	31.150	1.00 35.14	0
HETATM		Ō	нон	87	75.010	37.307	10.676	1.00 38.37	0
HETATM		Ō	НОН	88	91.471	42.227	35.142	1.00 46.93	0
HETATM		ō	нон	89	49.032	57.262	26.680	1.00 45.04	0
HETATM			НОН	90	58.819	35.855	26.787	1.00 33.51	0
HETATM		Ö	нон	91	66.610	35.147	36.987	1.00 41.70	Ó
HETATM		. 0	нон	92	66.423	29.073	14.771	1.00 36.38	0
HETATM		Ö	НОН	93	50.205	43.386	7.840	1.00 48.37	0
HETATM		0	нон	94	69.770	36.084	7.610	1.00 43.71	0
HETATM		Ö	нон	95	56.434	31.334	8.824	1.00 51.14	0
HETATM		o	нон	96	68.525	59.191	7.595	1.00 57.38	. 0
HETATM		0	нон	97	68.856	74.797	33.274	1.00 45.02	0
HETATM		Ö	нон	98	45.466	44.918	32.864	1.00 44.79	0
HETATM		Ö	нон	99	73.439	40.590	41.918	1.00 43.45	0
HETATM		Ö	нон	100	82.331	76.466	24.096	1.00 49.31	0
HETATM		Ö	нон	101	63.989	58.544	43.317	1.00 49.06	0
HETATM		0	нон	102	52.822	30.334	14.629	1.00 50.72	0
HETATM		Ö	нон	103	69.162	44.078	0.587	1.00 44.93	0
HETATM		Ö	нон	104	57.966	65.984	38.109	1.00 50.45	0
HETATM		o	нон	105	61.009	30.223	22.762	1.00 54.86	Ο·
HETATM		Ô	нон	106		40.912		1.00 51.59	- 0
HETATM		0	нон	107	83.364	55.951	16.129	1.00 38.90	0
HETATM		Ö	НОН	108	80.747	50.654	40.836	1.00 49.94	0
HETATM		Ö	нон	109	55.067	32.734	36.953	1.00 52.02	0
HETATM		Ö	нон	110	61.338	24.112	16.927	1.00 75.61	0
HETATM		Ö	нон	111	55.363	51.236	15.584	1.00 50.23	0
HETATM		Ö	нон	112	86.105	39.380	22.608	1.00 43.92	0
HETATM		0	нон	113	65.590	61.745	38.398	1.00 44.21	0
HETATM		0	нон	114	76.005	54.691	-0.953	1.00 60.80	0
HETATM		0	нон	115	63.472	78.599	34.826	1.00 49.03	0
HETATM		<i>'</i> 0	НОН	116	56.584	48.288	14.849	1.00 40.92	0
HETATM		0	нон	117	74.848	29.487	24.069	1.00 48.29	0
HETATM		0	нон	118	60.786	51.033	45.907	1.00 58.58	0
HETATM		0	нон	119	63.463	59.191	18.549	1.00 40.51	0
HETATM		Ö	нон	120	64.003	26.220	24.484	1.00 50.15	0
HETATM		0	нон	121	58.655	37.671	5.381	1.00 53.24	0
HETATM		0	нон	122	63.615	31.933	25.497	1.00 40.97	0
HETATM			нон	123	65.616	76.381	33.672	1.00 46.89	0
**** **** ***		_	22011						

HETATM	2863	0	HOH	124	55.158	44.415	39.591	1.00	56.77	0
HETATM	2864	0	HOH	125	75.132	48.039	35.838	1.00	43.66	0
HETATM	2865	0	HOH	126	65.816	28.316	26.676	1.00	42.04	0
HETATM	2866	0	HOH	127	54.208	52.470	12.608		47.30	0
HETATM	2867	0	HOH	128	53.242	30.460	11.276	1.00	68.84	0
HETATM	2868	0	HOH	129	60.726	33.090	34.181	1.00	47.71	0
HETATM	2869	0	HOH	130	64.010	40.397	3.202	1.00	52.21	0
HETATM	2870	0	HOH	131	77.504	52.228	0.017	1.00	50.80	0
HETATM	2871	0	HOH	132	69.804	61.883	38.293	1.00	46.95	0
HETATM	2872	0	HOH	133	45.792	41.736	13.068	1.00	47.40	0
HETATM	2873	0	НОН	134	50.939	33.262	11.744	1.00	43.38	0
HETATM	2874	0	НОН	135	76.312	35.442	27.267	1.00	53.79	0
HETATM		0	нон	136	62.510	56.249	46.266		55.19	0
HETATM		0	нон	137	73.706	35.590	8.247		48.59	0
HETATM		٥.	НОН	138	66.547	78.277	31.624		74.03	Ō
HETATM		0	нон	139	64.392	81.457	33.669		49.54	Ö
HETATM	_	0	нон	140	61.558	64.657	38.228		56.05	Ö
HETATM		Ō		141	96.215	46.485	27.601		49.93	ō
HETATM		·0 ·	НОН	142	61.787	33.565	27.109		49.84	ō
HETATM		0	нон	143	52.202	49.654	40.025		57.52	0
HETATM		0	нон	144	65.216	31.604	29.511		59.80	0
HETATM		0							57.79	0
			НОН	145	69.153	31.657	25.777		50.45	0
HETATM		0	НОН	146	60.092	41.511	39.950			
HETATM		0	НОН	147	74.800	33.112	28.850		67.42	0
HETATM		0	HOH	148	62.654	33.516	30.073		62.16	0
HETATM		0	нон	149	71.897	32.924	29.976		50.48	0
HETATM		0	НОН	150	56.804	34.357	25.133		46.97	0
HETATM		0	НОН	151	73.224	33.332	26.044		49.98	0
HETATM		0	НОН	152	62.549	28.935	25.883		63.89	0
HETATM		0	НОН	153	72.526	31.533	23.597		46.02	0
HETATM		0	НОН	154	55.400	54.063	40.193		51.55	0
HETATM		0	HOH	155	56.260	50.851	2.415		59.29	0
HETATM		0	HOH	156	59.029	24.830	22.198		60.82	0
HETATM		0	HOH	157	65.228	26.246	14.456		42.42	0
HETATM		0	HOH	158	74.086	29.603	13.669		44.88	0
HETATM	2898	0	HOH	159	71.012	57.900	14.425	1.00	49.16	0
HETATM		0	HOH	160	76.443	52.766	36.176	1.00	32.86	0
HETATM	2900	0	HOH	161	74.501	55.579	38.525	1.00	43.80	0
HETATM	2901	0.	HOH	162	68.390	53.333	47.198	1.00	57.30	0
HETATM	2902	0	HOH	163	66.068	54.957	48.273	1.00	52.03	0
HETATM	2903	0	HOH	164	90.274	44.981	34.515	1.00	42.74	0
HETATM	2904	0	HOH	165	92.357	46.800	32.648	1.00	50.13	0
HETATM	2905	0	HOH	166	87.411	55.494	37.249	1.00	49.75	0
HETATM	2906	0	HOH	167	65.234	66.995	39.283	1.00	56.66	0
HETATM	2907	0	HOH	168	75.023	62.880	19.374	1.00	43.60	0
HETATM	2908	0	HOH (	169	49.785	54.078	24.384	1.00	56.06	0
HETATM	2909	0	HOH	170	93.198	47.611	19.693	1.00	57.65	0
HETATM	2910	0	HOH	171	69.700	45.410	46.557	1.00	42.35	0
HETATM	2911	0	HOH	172	66.820	41.422	2.567	1.00	50.29	0
HETATM	2912	0	нон	173	87.119	47.913	13.662	1.00	52.23	0
HETATM		0	нон	174	72.571	61.611	21.232	1.00	34.11	0
HETATM		0	нон	175	81.561	38.698	24.061		46.29	0
HETATM		0	нон	176	70.615	32.679	38.298		45.72	0
HETATM		0	нон	177	53.945	58.607	38.141		50.80	0
HETATM		Ō	нон	178	69.562	62.885	21.604		28.51	0
HETATM		Ō	нон	179	69.716	68.855	36.042		48.11	ō
HETATM		Ō	нон	180	67.633	69.270	38.272		45.15	Ö
		-				0			-0.10	_

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CONECT 202 2519
CONECT 2519 202
CONECT 2693 2694 2695 2696 2697
CONECT 2694 2693
CONECT 2695 2693
CONECT 2696 2693 2698
CONECT 2697 2693
CONECT 2698 2696 2699
CONECT 2699 2698 2700 2715
CONECT 2700 2699 2701
CONECT 2701 2700 2702 2713
CONECT 2702 2701 2703 2712
CONECT 2703 2702 2704 2710
CONECT 2704 2703 2706
CONECT 2705 2706 2708
CONECT 2706 2704 2705 2707
CONECT 2707 2706
CONECT 2708 2705 2709 2710
CONECT 2709 2708
CONECT 2710 2703 2708 2711
CONECT 2711 2710 2712
CONECT 2712 2702 2711
CONECT 2713 2701 2714 2715
CONECT 2714 2713
CONECT 2715 2699 2713 2716
CONECT 2716 2715
CONECT 2717 2732 2734 2735
CONECT 2718 2719 2733
CONECT 2719 2718 2720 2725
CONECT 2720 2719 2721
CONECT 2721 2720 2722
CONECT 2722 2721 2738 2739
CONECT 2723 2728
CONECT 2724 2736
CONECT 2725 2719
CONECT 2726 2727 2735
CONECT 2727 2726 2728 2732
CONECT 2728 2723 2727 2729
CONECT 2729 2728 2730 2736
CONECT 2730 2729 2731 2733
CONECT 2731 2730 2732 2737
CONECT 2732 2717 2727 2731
CONECT 2733 2718 2730
CONECT 2734 2717
CONECT 2735 2717 2726
CONECT 2736 2724 2729
CONECT 2737 2731
CONECT 2738 2722
CONECT 2739 2722
MASTER
           550
                 0 3 14
                               18
                                       0
                                            0
                                                 6 2918 1 49
                                                                    39
END
Figure 13
P-UC 5440
Page 21
```

```
OXIDOREDUCTASE
                                                08-AUG-02
                                                            1MEW
HEADER
        INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
TITLE
TITLE
        2 TRITRICHOMONAS FOETUS WITH XMP AND NAD BOUND
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE;
COMPND 3 CHAIN: A;
COMPND 4 SYNONYM: IMP DEHYDROGENASE, IMPDH;
COMPND 5 EC: 1.1.1.205;
COMPND 6 ENGINEERED: YES
SOURCE MOL ID: 1;
SOURCE 2 ORGANISM SCIENTIFIC: TRITRICHOMONAS FOETUS;
SOURCE 3 GENE: IMPDH;
SOURCE 4 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE 5 EXPRESSION_SYSTEM_COMMON: BACTERIA;
SOURCE 6 EXPRESSION_SYSTEM_STRAIN: H712;
SOURCE 7 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE 8 EXPRESSION SYSTEM PLASMID: PBACE
KEYWDS ALPHA BETA BARREL
EXPDTA X-RAY DIFFRACTION
AUTHOR G.L.PROSISE, H.LUECKE
JRNL
         AUTH G.L.PROSISE, H.LUECKE
          TITL CRYSTAL STRUCTURE OF T. FOETUS INOSINE
JRNL
          TITL 2 MONOPHOSPHATE DEHYDROGENASE IN COMPLEX WITH
JRNL
         TITL 3 SUBSTRATE, COFACTOR, AND ANALOGS:STRUCTURAL BASIS
JRNL
         TITL 4 FOR THE RANDOM-IN ORDERED-OUT KINETIC MECHANISM
JRNL
          REF
                  TO BE PUBLISHED
JRNL
JRNL
           REFN
REMARK 1
REMARK
       2
REMARK
        2 RESOLUTION. 2.15 ANGSTROMS.
REMARK 3
REMARK 3 REFINEMENT.
REMARK 3 PROGRAM : CNS 1.1
                       : BRUNGER, ADAMS, CLORE, DELANO, GROS, GROSSE-
REMARK 3 AUTHORS
REMARK 3
                       : KUNSTLEVE, JIANG, KUSZEWSKI, NILGES, PANNU,
                        : READ, RICE, SIMONSON, WARREN
REMARK 3
REMARK 3
REMARK 3 REFINEMENT TARGET : ENGH & HUBER
REMARK
        3 DATA USED IN REFINEMENT.
REMARK
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.15
REMARK
            RESOLUTION RANGE LOW (ANGSTROMS) : 29.61
                                  (SIGMA(F)): 0.000
REMARK 3 DATA CUTOFF
REMARK 3 OUTLIER CUTOFF HIGH (RMS(ABS(F))) : NULL
REMARK 3 COMPLETENESS (WORKING+TEST) (%): 98.3
REMARK 3 NUMBER OF REFLECTIONS
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 CROSS-VALIDATION METHOD
                                            : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE
                               (WORKING SET) : 0.224
REMARK. 3 FREE R VALUE
                                            : 0.246
REMARK 3 FREE R VALUE TEST SET SIZE
                                         (%): 5.200
REMARK
        3 FREE R VALUE TEST SET COUNT
                                        : 1768
REMARK 3 ESTIMATED ERROR OF FREE R VALUE : 0.006
REMARK
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
```

```
REMARK 3 TOTAL NUMBER OF BINS USED
REMARK 3 TOTAL NUMBER OF BINS USED : 6

REMARK 3 BIN RESOLUTION RANGE HIGH (A) : 2.15

REMARK 3 BIN RESOLUTION RANGE LOW (A) : 2.28
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 95.80
REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 5092
REMARK 3 BIN R VALUE
                               (WORKING SET) : 0.2580
REMARK 3 BIN FREE R VALUE
REMARK 3 BIN FREE R VALUE TEST SET SIZE (%): 5.00
REMARK 3 BIN FREE R VALUE TEST SET COUNT : 270
REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.017
ŔEMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 2635
REMARK 3 NUCLEIC ACID ATOMS REMARK 3 HETEROGEN ATOMS
REMARK 3 SOLVENT ATOMS
                                  : 164
REMARK 3
REMARK 3 B VALUES.
                              (A**2) : 28.80
REMARK 3 FROM WILSON PLOT
REMARK 3 MEAN B VALUE (OVERALL, A**2): 36.10
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : 0.00000
REMARK 3 B22 (A**2) : 0.00000
REMARK 3 B33 (A**2) : 0.00000
REMARK 3 B12 (A**2) : 0.00000
REMARK 3 B13 (A**2) : 0.00000
REMARK 3 B23 (A**2) : 0.00000
REMARK 3
REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM LUZZATI PLOT (A): 0.26
                                      (A) : 0.22
REMARK 3 ESD FROM SIGMAA
REMARK 3 LOW RESOLUTION CUTOFF
                                    (A) : 5.00
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT ^ (A) : 0.30
REMARK 3 ESD FROM C-V SIGMAA
                                      (A) : 0.28
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS (A): 0.006
REMARK 3 BOND ANGLES
                                (DEGREES) : 1.20
                           (DEGREES) : 1.20
(DEGREES) : 22.90
REMARK 3 DIHEDRAL ANGLES
REMARK 3 IMPROPER ANGLES
                                 (DEGREES) : 0.77
       3
REMARK
       3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK
       3
REMARK
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                               RMS
REMARK 3 MAIN-CHAIN BOND (A**2) : 0.780 ; 1.500
REMARK 3 MAIN-CHAIN ANGLE (A**2) : 1.410 ; 2.000
REMARK 3 SIDE-CHAIN BOND
                                      (A**2) : 0.900 ; 2.000
REMARK 3 SIDE-CHAIN ANGLE
                                      (A**2) : 1.480 ; 2.500
REMARK 3
REMARK 3 BULK SOLVENT MODELING.
REMARK 3 METHOD USED : FLAT MODEL
REMARK 3 KSOL : 0.38
REMARK 3 BSOL
                      : 41.94
REMARK 3
REMARK 3 NCS MODEL : NULL
```

```
REMARK 3
REMARK 3 NCS RESTRAINTS.
                                                   RMS SIGMA/WEIGHT
REMARK 3 GROUP 1 POSITIONAL (A): NULL; NULL
REMARK 3 GROUP 1 B-FACTOR (A**2): NULL; NULL
REMARK 3
REMARK 3 PARAMETER FILE 1 : PROTEIN REP.PARAM
REMARK 3 PARAMETER FILE 2 : PARAM.GNSOL
REMARK 3 PARAMETER FILE 3 : CIS_PEPTIDE.PARAM
REMARK 3 PARAMETER FILE 4 : XMPG.PAR
REMARK 3 PARAMETER FILE 5 : NAD_PROD.PAR
REMARK 3 PARAMETER FILE 6 : NULL
REMARK 3 TOPOLOGY FILE 1 : PROTEIN.TOP
REMARK 3 TOPOLOGY FILE 2 : XMPG.TOP
REMARK 3 TOPOLOGY FILE 3 : NAD_PROD.TOP
REMARK 3 TOPOLOGY FILE 4 : ION.TOP
REMARK 3 TOPOLOGY FILE 5 : TOPH GNSOL REMARK 3 TOPOLOGY FILE 6 : NULL REMARK 3 OTHER REFINEMENT REMARKS: NULL
REMARK 4
REMARK 4 1MEW COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 16-AUG-2002.
REMARK 100 THE RCSB ID CODE IS RCSB016859.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE
                                          : X-RAY DIFFRACTION
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRAREMARK 200 DATE OF DATA COLLECTION : 01-NOV-2000
REMARK 200 TEMPERATURE (KELVIN) : 100.0
                                      : 7.50
REMARK 200 PH
REMARK 200 NUMBER OF CRYSTALS USED
REMARK 200
REMARK 200 SYNCHROTRON
REMARK 200 RADIATION SOURCE : ALS
REMARK 200 BEAMLINE
                                     : ALS
REMARK 200 BEAMLINE : 5.0.2
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A): 1.00
                                      : NULL
REMARK 200 MONOCHROMATOR
REMARK 200 OPTICS
                                           : NULL
REMARK 200
REMARK 200 DETECTOR TYPE : CCD REMARK 200 DETECTOR MANUFACTURER : ADSC QUANTUM 4
REMARK 200 DETECTOR TYPE
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE : SCALEPACK
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 33857
REMARK 200 RESOLUTION RANGE HIGH (A): 2.150
REMARK 200 RESOLUTION RANGE LOW (A): 50.000
REMARK 200 REJECTION CRITERIA (SIGMA(I)): 0.000
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE
                                      (%) : 98.4
REMARK 200 DATA REDUNDANCY
                                       : 5.400
REMARK 200 R MERGE
                                       (I) : 0.08000
REMARK 200 R SYM
                                       (I) : NULL
REMARK 200 <I/SIGMA(I) > FOR THE DATA SET : 19.0000
```

```
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.15
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.19
REMARK 200 COMPLETENESS FOR SHELL (%): 95.9 REMARK 200 DATA REDUNDANCY IN SHELL : NULL
REMARK 200 R MERGE FOR SHELL
REMARK 200 R SYM FOR SHELL
                                              (I) : 0.58000
                                             (I) : NULL
REMARK 200 <I/SIGMA(I) > FOR SHELL
                                                  : 2.200
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: FOURIER SYNTHESIS
REMARK 200 SOFTWARE USED: CNS
REMARK 200 STARTING MODEL: PDB ENTRY 1AK5
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: SODIUM MALONATE, TRIS, 2-
REMARK 280 MERCAPTOETHANOL, EDTA, GLYCEROL
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 4 3 2
REMARK 290
REMARK 290
                 SYMOP
                           SYMMETRY
REMARK 290
                 NNNMMM OPERATOR
                1555 X,Y,Z
REMARK 290 1555 X,Y,Z
REMARK 290 2555 -X,-Y,Z
REMARK 290 3555 -X,Y,-Z
REMARK 290 4555 X,-Y,-Z
REMARK 290 5555 Z,X,Y
REMARK 290 6555 Z,-X,-Y
REMARK 290 7555 -Z,-X,Y
REMARK 290 8555 -Z,X,-Y
REMARK 290 9555 Y,Z,X
REMARK 290 10555 -Y,Z,-X
REMARK 290 11555 Y,-Z,-X
REMARK 290 11555 -Y,-Z,-X
REMARK 290
                12555 -Y, -Z, X
REMARK 290
REMARK 290
                 13555 Y,X,-Z
              14555 -Y,-X,-Z
15555 Y,-X,Z
16555 -Y,X,Z
REMARK 290
REMARK 290
REMARK 290
REMARK 290 17555 X,Z,-Y
             18555 -X,Z,Y
19555 -X,-Z,Y
20555 X,-Z,Y
REMARK 290
REMARK 290
                           -X,-Z,-Y
REMARK 290
REMARK 290
                  21555 Z,Y,-X
REMARK 290 22555 Z,-Y,X
REMARK 290
                23555 -Z,Y,X
               24555 -Z,-Y,-X
REMARK 290
REMARK 290
              WHERE NNN -> OPERATOR NUMBER
REMARK 290
                 MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290
```

TABLE 5 250 -

REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY REMARK 290 RELATED MOLECULES. REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 REMARK 290 SMTRY2 2 · 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 0.00000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 

 REMARK 290
 SMTRY2
 10
 0.000000
 0.000000
 1.000000
 0.00000

 REMARK 290
 SMTRY1
 11
 0.000000
 1.000000
 0.000000
 0.00000

 REMARK 290
 SMTRY2
 11
 0.000000
 0.000000
 -1.000000
 0.00000

 REMARK 290 SMTRY3 11 -1.000000 0.000000 0.000000 REMARK 290 SMTRY1 12 0.000000 -1.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 REMARK 290 SMTRY2 12 0.000000 0.000000 -1.000000 REMARK 290 SMTRY3 12 1.000000 0.000000 0.000000 REMARK 290 SMTRY3 12 1.000000 0.000000 0.000000 REMARK 290 SMTRY1 13 0.000000 1.000000 0.000000 REMARK 290 SMTRY1 13 0.000000 1.000000 0.000000 REMARK 290 SMTRY2 13 1.000000 0.000000 0.000000 REMARK 290 SMTRY1 14 0.000000 -1.000000 0.000000 REMARK 290 SMTRY2 14 -1.000000 0.000000 0.000000 REMARK 290 SMTRY2 14 -1.000000 0.000000 0.000000 0.000000 | 0.00000 | 0.00000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.0000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.0000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.0000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.0000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.0000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.0000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.0000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.0000000 | 0.0000000 | 0.0000000 | 0.0000000 | 0.0000000 | 0.0000000 0.00000 REMARK 290 SMTRY3 17 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY1 18 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 18 0.000000 0.000000 1.000000 0.00000

```
REMARK 290 SMTRY3 18 0.000000 1.000000 0.000000
                                                                                                             0.00000
REMARK 290 SMTRY1 19 -1.000000 0.000000 0.000000
                                                                                                               0.00000
                     SMTRY2 19 0.000000 0.000000 -1.000000
                                                                                                                0.00000
REMARK 290
REMARK 290 SMTRY3 19 0.000000 -1.000000 0.000000 REMARK 290 SMTRY1 20 1.000000 0.000000 0.000000
                                                                                                                0.00000
                                                                                                       0.00000
REMARK 290 SMTRY2 20 0.000000 0.000000 -1.000000
REMARK 290 SMTRY3 20 0.000000 1.000000 0.000000
                                                                                                                0.00000
REMARK 290 SMTRY1 21 0.000000 0.000000 1.000000
                                                                                                             0.00000
REMARK 290 SMTRY2 21 0.000000 1.000000 0.000000
REMARK 290 SMTRY2 23 0.000000 1.000000 0.000000
                                                                                                              0.00000
REMARK 290 SMTRY3 23 1.000000 0.000000 0.000000
                                                                                                              0.00000
 REMARK 290 SMTRY1 24 0.000000 0.000000 -1.000000
REMARK 290 SMTRY2 24 0.000000 -1.000000 0.000000 REMARK 290 SMTRY3 24 -1.000000 0.000000 0.000000
                                                                                                             0.00000
                                                                                                              0.00000
 REMARK 290
 REMARK 290 REMARK: NULL
 REMARK 300 BIOMOLECULE: 1
 REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
 REMARK 300 WHICH CONSISTS OF 1 CHAIN(S). SEE REMARK 350 FOR
 REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
 REMARK 350
 REMARK 350 GENERATING THE BIOMOLECULE
 REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
 REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
 REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
 REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
 REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
 REMARK 350
 REMARK 350 BIOMOLECULE: 1
 REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
 REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000
                                                                                                               0.00000
 REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000
                                                                                                               0.00000
| COUNTY | C
 REMARK 350 BIOMT1 4 0.000000 -1.000000 0.000000
                                                                                                              153.82700
 REMARK 350 BIOMT2 4 1.000000 0.000000 0.000000
                                                                                                             0.00000
 REMARK 350 BIOMT3 4 0.000000 0.000000 1.000000
                                                                                                               0.00000
 REMARK 465
 REMARK 465 MISSING RESIDUES
 REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
 REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
 REMARK 465 IDENTIFIER; SSSEO=SEQUENCE NUMBER; I=INSERTION CODE.)
 REMARK 465
 REMARK 465 M RES C SSSEQI
 REMARK 465 MET A 1
REMARK 465 GLY A 102
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REMARK	465	PHE A	103
REMARK	465	VAL A	104
REMARK	465	VAL A	105
REMARK	465	SER A	106
REMARK	465	ASP A	107
REMARK	465	SER A	108
REMARK	465	ASN A	109
REMARK	465	VAL A	110
REMARK	465	LYS A	111
REMARK	465	PRO A	112
REMARK	465	ASP A	113
REMARK	465	GLN A	114
REMARK	465	THR A	115
REMARK	465	PHE A	116
REMARK	465	ALA A	117
REMARK	465	ASP A	118
REMARK	465	VAL A	119
REMARK	465	LEU A	120
REMARK	465	ALA A	121
REMARK	465	ILE A	122
REMARK	465	SER A	123
REMARK	465	GLN A	124
REMARK	465	ARG A	125
REMARK	465	THR A	126
REMARK	465	THR A	127
REMARK	465	HIS A	128
REMARK	465	ASN A	129
REMARK	465	THR A	130
REMARK	465	VAL A	131
REMARK	465	ALA A	132
REMARK	465	VAL A	133
REMARK	465	THR A	134
REMARK	465	ASP A	135
REMARK	465	ASP A	136
REMARK	465	GLY A	137
REMARK	465	THR A	
REMARK	465		138 139
REMARK	465		140
REMARK	465	HIS A GLY A	141
REMARK			
REMARK	465 465		142
REMARK	465		143
REMARK	465	LEU A GLY A	144 145
REMARK			
REMARK	465	LEU A	146
	465	VAL A	147
REMARK REMARK	465	THR A	148
	465	GLN A	149
REMARK	465	ARG A	150
REMARK	465	ASP A	151
REMARK	465	TYR A	152
REMARK	465	PRO A	153
REMARK	465 '	ILE A	154
REMARK	465	ASP A	155
REMARK	465	LEU A	156
REMARK	465	THR A	157
REMARK	465	GLN A	158
REMARK	465	THR A	159

REMARK	465	GLU A	160
REMARK	465	THR A	161
REMARK	465	LYS A	162
REMARK	465	VAL A	163
REMARK	465	SER A	164
REMARK	465	ASP A	165
REMARK	465	MET A	166
REMARK	465	MET A	167
REMARK	465	THR A	168
REMARK	465	PRO A	169
REMARK	465	PHE A	170
REMARK	465	SER A	171
REMARK	465	LYS A	172
REMARK	465	LEU A	173
REMARK	465	VAL A	174
REMARK	465	THR A	175
REMARK	465	ALA A	176
REMARK	465	HIS A	177
REMARK	465	GLN A	178
REMARK	465	ASP A	179
REMARK	465	THR A	180
REMARK	465	LYS A	181
REMARK	465	LEU A	182
	465	SER A	183
REMARK	465	GLU A	184
REMARK	465	ALA A	185
REMARK	465	ASN A	186
REMARK	465	LYS A	187
REMARK	465	ILE A	188
REMARK	465	ILE A	189
REMARK	465	TRP A	190
REMARK	465	GLU A	191
REMARK	465	LYS A	192
REMARK	465	LYS A	193
REMARK		LEU A	194
REMARK		ASN A	195
REMARK	465	ALA A	196
REMARK	465	LEU A	197
REMARK	465.	PRO A	198
REMARK	465	ILE A	199
REMARK	465	ILE A	200
REMARK	465	ASP A	201
REMARK	465	ASP A	202
REMARK	465	ASP A	203
REMARK	465	GLN A	204
REMARK	465	HIS A	205
REMARK	465	LEU A	206
REMARK	465	ARG A	207
REMARK	465	TYR A	208
REMARK	465	ILE A	209
REMARK	465	VAL A	210
REMARK	465	PHE A	211
REMARK	465	ARG A	211
REMARK	465	LYS A	213
REMARK	465	ASP A	214
REMARK	465	TYR A	214
REMARK	465	ASP A	216

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REMARK 465
               ARG A
                        217
REMARK 465
               SER A
                        218
REMARK 465
               GLN A
                        219
REMARK 465
               VAL A
                        220
REMARK 465
               CYS A
                        221
REMARK 465
               ILE A
                        318
REMARK 465
               CYS A
                        319
REMARK 465
               ILE A
                        320
REMARK 465
               THR A
                        321
REMARK 465
               GLN A
                        417
REMARK 465
               ARG A
                        418
REMARK 465
               TYR A
                        419
REMARK 465
               ASP A
                        420
REMARK 465
               LEU A
                        421
REMARK 465
               GLY A
                        422
REMARK 465
               GLY A
                        423
               LYS A
REMARK 465
                        424
REMARK 465
               GLN A
                        425
REMARK 465
               LYS A
                        426
REMARK 465
               LEU A
                        427
REMARK 465
               SER A
                        428
REMARK 465
               PHE A
                        429
REMARK 465
               GLU A
                        430
REMARK 465
               VAL A
                        484
REMARK 465
               GLU A
                        485
REMARK 465
               GLY A
                        486
REMARK 465
               GLY A
                        487
REMARK 465
               ALA A
                        488
               HIS A
REMARK 465
                        489
               ASP A
REMARK 465
                        490
REMARK 465
               VAL A
                        491
REMARK 465
               ILE A
                        492
REMARK 465
               VAL A
                        493
               LYS A
REMARK 465
                        494
               ASP A
REMARK 465
                        495
REMARK 465.
               ARG A
                        496
REMARK 465
               ILE A
                        497
REMARK 465
               ASN A
                        498
REMARK 465
               ASP A
                        499
REMARK 465
               TYR A
                        500
REMARK 465
               HIS A
                        501
REMARK 465
               PRO A
                        502
               LYS A
REMARK 465
                        503
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE: .
REMARK 500 FORMAT: (10X, I3, 1X, 2(A3, 1X, A1, I4, A1, 1X, A4, 3X), F6.3)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
```

```
REMARK 500 M RES CSSEQI ATM1
                               RES CSSEQI ATM2
 REMARK 500 VAL A 62 CB
                               VAL A 62 CA
                                                0.036
 REMARK 500 MET A 92
                         CE
                               MET A 92
                                          SD
                                                -0.071
 REMARK 500 MET A 458 CE
                               MET A 458 SD
                                                0.037
 REMARK 500
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY
 REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
 REMARK 500
 REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
 REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
 REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
 REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
 REMARK 500
 REMARK 500 STANDARD TABLE:
 REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3 (1X, A4, 2X), 12X, F5.1).
 REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
 REMARK 500 M RES CSSEQI ATM1 ATM2 ATM3
 REMARK 500 GLY A 20 N - CA - C
                                         ANGL. DEV. = -7.9 DEGREES
 REMARK 500 ILE A 27 N - CA - C
                                          ANGL. DEV. = -9.5 DEGREES
 REMARK 500 PHE A 266 N - CA - C ANGL. DEV. = -7.5 DEGREES
 REMARK 500 GLY A 312 N - CA - C ANGL. DEV. = 7.8 DEGREES
 REMARK 500 LYS A 472 N - CA - C ANGL. DEV. = 8.0 DEGREES
 REMARK 500 LYS A 474 N - CA - C ANGL. DEV. = -8.4 DEGREES
            LEU A 477 N - CA - C ANGL. DEV. = -8.5 DEGREES
 REMARK 500
 REMARK 900
 REMARK 900 RELATED ENTRIES
 REMARK 900 RELATED ID: 1AK5 RELATED DB: PDB
 REMARK 900 INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM.
 REMARK 900 TRITRICHOMONAS FOETUS
 REMARK 900 RELATED ID: 1ME7 RELATED DB: PDB
 REMARK 900 1ME7 CONTAINS THE SAME PROTEIN WITH RVP AND MOA BOUND
 REMARK 900 RELATED ID: 1ME8 RELATED DB: PDB
 REMARK 900 1ME8 CONTAINS THE SAME PROTEIN WITH RVP BOUND
 REMARK 900 RELATED ID: 1ME9 RELATED DB: PDB
 REMARK 900 1ME9 CONTAINS THE SAME PROTEIN WITH IMP BOUND
 REMARK 900 RELATED ID: 1MEH RELATED DB: PDB
 REMARK 900 1MEH CONTAINS THE SAME PROTEIN WITH IMP AND MOA BOUND
 REMARK 900 RELATED ID: 1MEI RELATED DB: PDB
 REMARK 900 1MEI CONTAINS THE SAME PROTEIN WITH XMP AND MYCOPHENOLIC
 REMARK 900 ACID BOUND
 DBREF 1MEW A 1 503 SWS
                               P50097
                                       IMDH TRIFO
                                                         1
 SEQRES 1 A 503 MET ALA LYS TYR TYR ASN GLU PRO CYS HIS THR PHE ASN
         2 A 503 GLU TYR LEU LEU ILE PRO GLY LEU SER THR VAL ASP CYS
 SEQRES
        3 A 503 ILE PRO SER ASN VAL ASN LEU SER THR PRO LEU VAL LYS
 SEORES
 SEQRES 4 A 503 PHE GLN LYS GLY GLN GLN SER GLU ILE ASN LEU LYS ILE
 SEQRES 5 A 503 PRO LEU VAL SER ALA ILE MET GLN SER VAL SER GLY GLU
 SEQRES 6 A 503 LYS MET ALA ILE ALA LEU ALA ARG GLU GLY GLY ILE SER
 SEQRES 7 A 503 PHE ILE PHE GLY SER GLN SER ILE GLU SER GLN ALA ALA
 SEQRES 8 A 503 MET VAL HIS ALA VAL LYS ASN PHE LYS ALA GLY PHE VAL
 SEQRES 9 A 503 VAL SER ASP SER ASN VAL LYS PRO ASP GLN THR PHE ALA
 SEQRES 10 A 503 ASP VAL LEU ALA ILE SER GLN ARG THR THR HIS ASN THR
 SEQRES 11 A 503 VAL ALA VAL THR ASP ASP GLY THR PRO HIS GLY VAL LEU
 SEQRES 12 A 503 LEU GLY LEU VAL THR GLN ARG ASP TYR PRO ILE ASP LEU
 SEQRES 13 A 503 THR GLN THR GLU THR LYS VAL SER ASP MET MET THR PRO
 SEQRES 14 A 503 PHE SER LYS LEU VAL THR ALA HIS GLN ASP THR LYS LEU
```

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SEORES 15 A 503 SER GLU ALA ASN LYS ILE ILE TRP GLU LYS LYS LEU ASN
       16 A 503 ALA LEU PRO ILE ILE ASP ASP GLN HIS LEU ARG TYR
SEORES
SEQRES 17 A 503 ILE VAL PHE ARG LYS ASP TYR ASP ARG SER GLN VAL CYS
SEQRES 18 A 503 HIS ASN GLU LEU VAL ASP SER GLN LYS ARG TYR LEU VAL
SEGRES 19 A 503 GLY ALA GLY ILE ASN THR ARG ASP PHE ARG GLU ARG VAL
SEORES 20 A 503 PRO ALA LEU VAL GLU ALA GLY ALA ASP VAL LEU CYS ILE
SEQRES 21 A 503 ASP SER SER ASP GLY PHE SER GLU TRP GLN LYS ILE THR
SEQRES 22 A 503 ILE GLY TRP ILE ARG GLU LYS TYR GLY ASP LYS VAL LYS
SEORES
      23 A 503 VAL GLY ALA GLY ASN ILE VAL ASP GLY GLU GLY PHE ARG
SEORES
       24 A
             503 TYR LEU ALA ASP ALA GLY ALA ASP PHE ILE LYS ILE GLY
SEQRES 25 A
            503
                 ILE GLY GLY GLY SER ILE CYS ILE THR ARG GLU GLN LYS
SEQRES 26 A 503 GLY ILE GLY ARG GLY GLN ALA THR ALA VAL ILE ASP VAL
SEQRES 27 A 503 VAL ALA GLU ARG ASN LYS TYR PHE GLU GLU THR GLY ILE
SEORES 28 A 503 TYR ILE PRO VAL CYS SER ASP GLY GLY ILE VAL TYR ASP
SEQRES 29 A 503 TYR HIS MET THR LEU ALA LEU ALA MET GLY ALA ASP PHE
SEQRES 30 A 503 ILE MET LEU GLY ARG TYR PHE ALA ARG PHE GLU GLU SER
SEQRES 31 A 503 PRO THR ARG LYS VAL THR ILE ASN GLY SER VAL MET LYS
SEQRES 32 A 503 GLU TYR TRP GLY GLU GLY SER SER ARG ALA ARG ASN TRP
SEQRES 33 A 503 GLN ARG TYR ASP LEU GLY GLY LYS GLN LYS LEU SER PHE
SEQRES 34 A 503 GLU GLU GLY VAL ASP SER TYR VAL PRO TYR ALA GLY LYS
SEQRES 35 A 503 LEU LYS ASP ASN VAL GLU ALA SER LEU ASN LYS VAL LYS
SEQRES 36 A 503 SER THR MET CYS ASN CYS GLY ALA LEU THR ILE PRO GLN
SEQRES 37 A 503 LEU GLN SER LYS ALA LYS ILE THR LEU VAL SER SER VAL
SEQRES 38 A 503 SER ILE VAL GLU GLY GLY ALA HIS ASP VAL ILE VAL LYS
SEQRES 39 A 503 ASP ARG ILE ASN ASP TYR HIS PRO LYS
       K A 900
HET
                      1
    XMP
HET
             602
                      24
HET
      NAD
             987
                     44
HETNÁM
            K POTASSIUM ION
HETNAM
          XMP XANTHOSINE-5'-MONOPHOSPHATE
HETNAM .
          NAD NICOTINAMIDE-ADENINE-DINUCLEOTIDE
HETSYN
          XMP 5--MONOPHOSPHATE-9-BETA-D-RIBOFURANOSYL XANTHINE
FORMUL
           K
                 K1 1+
        2
FORMUL
        3 XMP
                  C10 H14 N4 O9 P1 1+
FORMUL
        4 NAD
                 C21 H27 N7 O14 P2
FORMUL
        5
          HOH
                 *164(H2 O1)
HELIX
        1
            1 THR A
                      11 ASN A
                                 13
                                     5
                                                                        3
HELIX
        2
           2 ILE A
                      27
                         VAL A
                                 31 5
                                                                       · 5
                                 74 1
HELIX
        3
           3 GLY A
                      64
                        GLU A
                                                                       11
HELIX
        4
            4 SER A
                      85
                        ASN A
                                 98 1
                                                                       14
HELIX
        5
            5 ASP A
                    242 GLY A 254 1
                                                                       13
                    267 GLY A 282 1
HELIX
        6
           ·6 SER A
                                                                       16
HELIX
        7
            7 ASP A 283 VAL A 285 5
                                                                       3
            8 ASP A 294 GLY A 305 1
HELIX
        8
                                                                       12
            9 GLY A
                         GLY A 350 1
HELIX
       9
                    330
                                                                       21
HELIX
       10
           10 TYR A
                    363
                         MET A
                                373
                                                                       11
HELIX
       11
           11 GLY A
                    381
                         ARG A
                                386 1
                                                                        6
HELIX
       12
           12 LYS A 442
                         CYS A 461
                                                                       20
       13
HELIX
           13 THR A 465 ALA A 473 1
SHEET
       1
           A 2 TYR A 15 LEU A 17 0
SHEET
            A 2 ILE A 475 LEU A 477 -1
                                        0
                                           THR A 476
                                                         LEU A
                                                                16
SHEET
            B 2 THR A 35 PRO A 36 0
        1
SHEET
        2
            B 2 ASN A 49
                          LEU A 50 -1
                                        O LEU A 50
                                                      Ν
                                                         THR A
                                                                35
                          GLN A 41 0
SHEET
            C 2 PHE A 40
        1
SHEET
            C 2 ILE A 351
                          TYR A 352 -1
                                           TYR A 352
                                                         PHE A
                                                      N
                                                                40
SHEET
        1
            D 9 LEU A 54
                          SER A 56 0
SHEET
           D 9 ILE A 77
                          ILE A 80 1 O ILE A 77
                                                      N SER A
```

```
D 9 GLY A 235
                                                       N ILE A 80
SHEET
                           ILE A 238 1
                                       0
                                           GLY A 237
        3
SHEET
            D 9 VAL A 257
                           ILE A 260
                                     1
                                        0
                                           CYS A 259
                                                       N ILE A 238
            D 9 VAL A 287
                           ILE A 292
SHEET
                                     1
                                        0
                                           GLY A 288
                                                       N
                                                          LEU A 258
SHEET
            D 9 PHE A 308
                           ILE A 311
                                                          ALA A 289
        6
                                        0
                                           LYS A 310
                                                       N
                                     1
SHEET
        7
            D 9 VAL A 355
                           ASP A 358
                                     1
                                        0
                                           CYS A 356
                                                          ILE A 311
                                                       N
            D 9 PHE A 377
                           LEU A 380
SHEET
        8
                                     1
                                        0
                                           MET A 379
                                                       N
                                                          SER A 357
SHEET
        9
            D 9 LEU A 54
                           SER A 56' 1
                                        N
                                           VAL A 55
                                                          ILE A 378
SHEET
        1
            E 3 LYS A 394
                           ILE A 397
                                     0
SHEET
        - 2
            E 3 SER A 400
                           TRP A 406 -1
                                        O MET A 402
                                                          VAL A 395
                                                       N
SHEET
        3
            E 3 ASP A 434 PRO A 438 -1 O SER A 435
                                                       N TYR A 405
SSBOND
        1 CYS A
                  26
                       CYS A 459
CISPEP
        1 GLY A 290
                       ASN A 291
                                           0
                                                     1.02
       153.827 153.827 153.827 90.00 90.00 90.00 P 4 3 2
CRYST1
                                                                  24
           1.000000 0.000000 0.000000
ORIGX1
                                        0.00000
ORIGX2
           0.000000 1.000000 0.000000
                                              0.00000
           0.000000 0.000000 1.000000
ORIGX3 .
                                              0.00000
           0:006501 0.000000 0.000000
SCALE1
                                              0.00000
           0.000000 0.006501 0.000000
SCALE2
                                              0.00000
SCALE3
           0.000000 0.000000 0.006501
                                              0.00000
ATOM
                ALA A 2
         1 N
                              54.794 74.512 36.618 1.00 30.12
MOTA
         2 CA ALA A
                      2
                               55.518 73.408 35.927 1.00 29.62
                                                                          C
ATOM
         3 C
                ALA A 2
                               56.825 73.048
                                             36.643 1.00 30.02
                                                                          C
MOTA
         4 0
                ALA A 2
                              57.295
                                      73.782 37.518 1.00 28.78
                                                                          0
MOTA
         5 CB
               ALA A
                      2
                               55.807
                                      73.811
                                              34.492 1.00 29.41
                                                                          C
MOTA
         6 N
                LYS A
                        3
                               57.397
                                      71.908
                                              36.261 1.00 29.90
                                                                          N
         7
            CA
                LYS A
MOTA
                        3
                               58.649
                                      71.435
                                              36.834
                                                      1.00 30.45
                                                                          C
MOTA '
         8
            C
                LYS A
                       3
                               59.766
                                      71.663
                                              35.818
                                                      1.00 30.17
                                                                          C
MOTA
         9
                      3
            0
                LYS A
                              59.626
                                      71.311
                                              34.648 1.00 29.92
                                                                          0
ATOM
        10
            CB
                LYS A
                      3
                              58.564
                                      69.938
                                             37.150 1.00 31.27
                                                                          C
MOTA
        11
            CG
                LYS A
                      . 3
                              59.840
                                      69.374
                                              37.767 1.00 33.74
                                                                          С
ATOM
        12
            CD
                LYS A
                       3
                              59.988
                                      67.882
                                              37.515 1.00 35.82
                                                                          C
MOTA
        13
            CE
                LYS A
                        3
                              61.209
                                      67.325
                                              38.235 1.00 37.03
                                                                          C
MOTA
        14 NZ
                LYS A
                        3
                               62.422
                                      68.153
                                             38.000 1.00 37.77
                                                                          N
MOTA
        15 N
                TYR A
                               60.868
                                      72.249
                                              36.273 1.00 30.13
                        4
                                                                          N
ATOM .
        `16
           CA
                TYR A
                              62.022
                                      72.523
                                              35.421 1.00 30.22
                        4
                                                                          C
MOTA
        17
            С
                TYR A
                        4
                              63.218
                                      71.738
                                              35.939
                                                      1.00 30.80 . .
                                                                          C
MOTA
        18
           0
                TYR A
                        4
                               63.151
                                      71.131
                                              37.003
                                                      1.00 31.54
                                                                          0
                                     74.023
MOTA
        19
            CB
                TYR A
                        4
                               62.333
                                              35.429
                                                      1.00 29.07
                                                                          С
MOTA
        20 CG
                TYR A
                        4
                               61.238 74.845
                                              34.800 1.00 28.39
                                                                          C
ATOM
        21
            CD1 TYR A
                              61.148 74.974
                        4
                                              33.417
                                                      1.00 27.65
                                                                          C
        22 CD2 TYR A
MOTA
                               60.260
                        4
                                      75.464
                                              35.588 1.00 28.22
                                                                          C
MOTA
        23
           CE1 TYR A
                               60.106
                                      75.701
                                              32.827 1.00 27.89
                                                                          C
MOTA
           CE2 TYR A
        24
                        4
                               59.213
                                      76.192
                                             35.007
                                                      1.00 27.42
                                                                          C
MOTA
        25 CZ
                TYR A
                                      76.304
                        4
                               59.145
                                              33.629
                                                      1.00 27.38
                                                                          C
MOTA
        26
           OH
                TYR A
                                      77.005
                                                      1.00 27.02
                        4
                               58.116
                                              33.045
                                                                          0
MOTA
        27
            N
                TYR A
                                      71.749
                        5
                               64.313
                                              35.190
                                                      1.00 31.44
                                                                          N
ATOM
        28
           CA
                TYR A
                        5
                               65.508
                                      71.016
                                              35.597
                                                      1.00 32.16
                                                                          C
                            66.719
ATOM
        29
            C
                TYR A
                        5
                                      71.930
                                              35.741
                                                      1.00 32.66
                                                                          C
MOTA
        30
            0
                TYR A
                        5
                               66.779
                                      73.005
                                              35.142
                                                      1.00 32.67
                                                                          0
MOTA
        31
            CB
                TYR A
                        5
                               65.806
                                      69.894
                                                      1.00 31.56
                                              34.594
                                                                          C
ATOM
        32
            CG
                        5
                TYR A
                               64.679
                                      68.891
                                              34.466
                                                      1.00 31.13
                                                                          С
MOTA
        33
            CD1 TYR A
                        5
                               63.511
                                      69.212
                                              33.777
                                                      1.00 30.96
                                                                          C
MOTA
        34
           CD2 TYR A
                        5
                               64.763
                                      67.634
                                             35.073
                                                      1.00 31.04
                                                                          C
MOTA
        35 CE1 TYR A
                       5
                              62.453
                                                                          C
                                      68.311
                                              33.694
                                                      1.00 30.92
MOTA
        36 CE2 TYR A
                        5
                              63.713
                                      66.726
                                              34.997
                                                      1.00 30.33
                                                                          С
MOTA
        37 CZ
                      5
                                      67.071
                TYR A
                              62.559
                                              34.307
                                                      1.00 31.08
                                                                          С
                      5
ATOM
        38 OH
                TYR A
                              61.504 66.189 34.242 1.00 30.49
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MOTA		39	N	ASN	A	6	67.681	71.495	36.545	1.00 33.45		N
ATOM		40	CA	ASN	Α	6	68.889	72.271	36.796	1.00 34.17		C
MOTA		41	С	ASN	A	6	69.829	72.350	35.596	1.00 33.77	•	С
ATOM		42	0	ASN	Α	6	70.505.	73.357	35.404	1.00 34.57		0
MOTA		43	CB	ASN	A	6	69.635	71.684	37.997	1.00 36.09	•	C
MOTA		44	CG	ASN	A	6	68.893	71.902	39.311	1.00 38.01	•	C
MOTA		45	OD1	ASN	A	6	69.083	71.156	40.276	1.00 39.34		. 0
MOTA		46		ASN		6	68.054	72.936	39.356	1.00 38.72		N
MOTA		47	N	GLU		7	69.868	71.296	34.786	1.00 32.81		N
MOTA		48	CA	GLU		7	70.752	71.262	33.623	1.00 31.44		C
ATOM	•	49	С	GLU		. 7	70.016	70.880	32.351	1.00 30.04		C
ATOM		50	0	GLU		7	69.016	70.166	32.393	1.00 29.37		0
ATOM		51	CB	GLU		7	71.870	70.238	33.840	1.00 32.95		C
ATOM		52	CG	GLU		7	72.811	70.511	35.009	1.00 34.80		С
ATOM		53	CD	GLU		7	73.665	71.758	34.814	1.00 36.26		Ć
ATOM		54		GLU		7	74.098	72.025	33.667	1.00 37.11		ō
ATOM		55		GLU		7	73.919	72.463	35.816	1.00 37.12		ō
MOTA		56	N	PRO		8	70.505	71.353	31.193	1.00 28.73		N
ATOM		57	CA	PRO		8	69.854	71.015	29.925	1.00 27.94		C
ATOM		58	C	PRO		8	70.216	69.567	29.597	1.00 27.34		C
ATOM		59	0	PRO		8	71.198	69.043	30.127	1.00 26.26		0
										1.00 20.26		C
ATOM		60	CB	PRO		8	70.481	72.004	28.945			C
ATOM		61	CG	PRO		8 .	71.873	72.153	29.484	1.00 27.96		
MOTA		62	CD	PRO		8	71.641	72.268	30.975	1.00 28.51		C
MOTA		63	N	CYS		9	69.432	68.918	28.742	1.00 26.44		N
MOTA		64	·CA	CYS		9	69.730	67.539	28.375	1.00 26.06		C
MOTA		65	C	CYS		9	70.788	67.503	27.266	1.00 25.59		C
MOTA		66	0	CYS		9	70.978	68.484	26.546	1.00 25.32		0
MOTA		67	CB	ĊYS		9	68.452	66.801	27.950	1.00 26.04		C
ATOM		68	SG	CYS		9	67.458	67.585	26.659	1.00 27.03		S
MOTA		69	N	HIS		10	71.478	66.373	27.146	1.00 25.08		N
ATOM		70	CA	HIS		10	72.545	66.203	26.163	1.00 24.94		C
MOTA		71	C .	HIS		10	72.398	64.914	25.351	1.00 25.14		С
ATOM		72	0	HIS		10	71.761	63.957	25.789	1.00 24.67		0
MOTA		73	CB	HIS		10 .	73.900	66.172	26.875	1.00 25.17		С
ATOM		74	CG	HIS		10	74.154	67.356		1.00 25.33		С
MOTA		75		HIS		. 10	74.603	68.565	27.269	1.00 25.05		N
MOTA		76		HIS		10	74.016	67.517	29.092	1.00 25.00		C
ATOM		77		HIS		10	74.731	69.419	28.267	1.00 24.83		C
MOTA		78	NE2	HIS	А	10	74.381	68.807	29.385	1.00 25.63		N
MOTA	·	79	N	THR	Α	11	73.012	64.905	24.174	1.00 25.28		N
MOTA		80	CA	THR		11	72.988	63.760	23.268	1.00 26.09		С
MOTA		81	C	THR	A	11	74.336	63.045	23.334	1.00 25.82		С
MOTA		82	0	THR	Α	11	75.309	63.600	23.852	1.00 25.75	-	0
MOTA		83	CB	THR		11	72.759	64.210	21.814	1.00 26.08		C
ATOM		84	OG1	THR	A	11	73.768	65.160	21.456	1.00 27.99		0
MOTA		85	CG2	THR	A	11	71.401	64.859	21.655	1.00 26.96		C
ATOM		86	N	PHE	Α	12	74.391	61.825	22.803	1.00 26.03		N
ATOM		87	CA	PHE	A	12	75.618	61.028	22.798	1.00 26.92		C
ATOM		88	С	PHE	A	12	76.820	61.750	22.185	1.00 27.61		С
MOTA		89	0	PHE	A	12	77.957	61.556	22.625	1.00 27.79	•	0
MOTA		90	CB	PHE		12	75.400	59.710	22.050	1.00 26.64	,	C
MOTA		91	CG	PHE		12	74.493	58.740	22.763	1.00 26.79		C
MOTA		92		PHE		12	74.631	58.510	24.131	1.00 26.53	,	С
MOTA		93		PHE		12	73.533	58.023	22.056	1.00 26.50		C
MOTA		94		PHE		12	73.826	57.577	24.787	1.00 26.96		C
ATOM		95		PHE		12	72.723	57.085	22.700	1.00 27.06		C
			_									

ATOM	96	CZ	PHE	Α	12	72.870	56.861	24.072	1.00 26.55	С
ATOM	97	N	ASN	А	13	76.567	62.569	21.167	1.00 28.01	N
ATOM	98	CA	ASN		13	77.614	63.330	20.484	1.00 28.79	C
ATOM	99	C	ASN		13	78.353	64.309	21,392	1.00 28.20	C
MOTA	100	0	ASN		13	79.409	64.822	21.027	1.00 28.50	0
	101	CB	ASN		13	77.013	64.115	19.316	1.00 30.83	C
ATOM										C
ATOM	102	CG	ASN		13	76.925	63.299	18.041	1.00 33.42	
ATOM	103		ASN		13	76.014	63.490	17.235	1.00 35.66	0
ATOM.	104	ND2	ASN		13	7.7.883	62.400	17.838	1.00 34.84	N
MOTA	105	N	GLU		14	77.799	64.580	22.568	1.00 27.32	N
ATOM	106	CA	GLU	A	14	78.422	65.520	23.494	1.00 26.81	C
MOTA	107	C	GLU	A	14	79.333	64.863	24.528	1.00 26.48	C
MOTA	108	0	GLU	Α	14	79.794	65.524	25.462	1.00 26.71	0
MOTA	109	CB	GLU	Α	14	77.342	66.330	24.215	1.00 26.50	C
ATOM	110	CG	GLU	٠.	14	76.448	67.124	23.283	1.00 26.18	С
ATOM	111	CD	GLU		14	75.339	67.860	24.014	1.00 25.91	С
ATOM	112	OE1			14	75.643	68.736	24.848	1.00 25.89	0
ATOM	113		GLU		14	74.158	67.559	23.750	1.00 25.85	Ō
ATOM	114	N	TYR		15	79.610	63.576		1.00 25.89	N
									1.00 25.89	C
ATOM	115	CA	TYR		15	80.454	62.880	25.325		
ATOM	116	C	TYR		15	81.647	62.145	24.733	1.00 25.92	C
MOTA	117	0	TYR		15	81.652	61.758	23.562	1.00 25.82	0
MOTA	118	CB	TYR		15	79.616	61.876	26.122	1.00 25.79	С
MOTA	119	CG	TYR		15	78.551	62.505	26.986	1.00 26.02	C
MOTA	120	CD1			15	78.814	62.856	28.310	1.00 25.94	C
MOTA	121	CD2	TYR		15	77.276	62.757	26.475	1.00 25.51	C
MOTA	122	CE1	TYR	A	15	77.831	63.440	29.107	1.00 26.32	С
MOTA	123	CE2	TYR	Α	15	76.296	63.339	27.256	1.00 25.69	С
ATOM	124	CZ	TYR	A	15	76.574	63.678	28.567	1.00 26.16	С
ATOM	125	OH	TYR	A	15	75.595	64.268	29.328	1.00 27.92	0
ATOM	126	N	LEU	A	16	82.659	61.958	25.571	1.00 25.68	N
MOTA	127	CA	LEU		16	83.857	61.221	25.201	1.00 25.59	С
ATOM	128	C	LEU		16	84.240	60.398	26.421	1.00 25.18	С
ATOM	129	Ō	LEU		16	83.879	60.741	27.545	1.00 23.99	0
ATOM	130	CB	LEU		16	85.011	62.163	24.835	1.00 25.74	C
ATOM	131	CG	LEU		16	84.924	62.928	23.513	1.00 26.58°	C
ATOM	132		LEU		16	86.164	63.782	23.349	1.00 26.64	C
								22.355	1.00 26.82	,C
MOTA	133		LEU		16	84.802	61.955			
ATOM	134	N G7	LEU		17	84.955	59.304	26.193	1.00 25.52	N
ATOM	135	CA	LEU		17	85.403	58.444	27.281	1.00 25.75	C
ATOM .	136	C	LEU		17	86.873	58.726	27.569	1.00 25.91	C
MOTA	137	0	LEU		17	87.685	58.859	26.649	1.00 26.05	0
MOTA	138	CB	LEU		17	85.236	56.973	26.898	1.00 25.70	C
ATOM	139	CG	LEU		17	83.811	56.418	26.904	1.00 25.75	C
MOTA	140		LEU		17	83.715	55.203	25.988	1.00 25.70	C
MOTA	141	CD2	LEU		17	83.422	56.062	28.330	1.00 24.96	C
MOTA	142	N	ILE	Α	18	87.207	58.841	28.848	1.00 26.13	N
MOTA	143	CA	ILE	Α	18	88.584	59.070	29.247	1.00 26.23	C
ATOM	144	C	ILE	A	18	89.125	57.707	29.665	1.00 26.76	C
MOTA	145	0	ILE		18	88.568	57.054	30.547	1.00 26.89	0
MOTA	146	CB	ILE		18	8.8.657	60.077	30.408	1.00 26.10	C
ATOM	147		ILE		18	88.213	61.457	29.896	1.00 25.77	C
ATOM	148		ILE		18	90.078	60.122	30.983	1.00 25.02	C.
ATOM	149		ILE		18	88.079	62.511	30.963	1.00 27.03	C
ATOM	150	Ŋ	PRO		19	90.209	57.251	29.016	1.00 27.09	N
MOTA		CA	PRO			90.209	55.949	29.016	1.00 27.09	C
	151				19					C
MOTA	152	С	PRO	A	19	91.121	55.680	30.792	1.00 27.03	Ċ

MOTA	153	0	PRO	A	19	91.403	56.595	31.562	1.00 27.37	0
ATOM	154	CB	PRO	Α	19	92.098	55.960	28.477	1.00 27.80	C
ATOM	155	CG	PRO	Α	19	91.703	56.803	27.280	1.00 27.76	C
ATOM	156	CD	PRO	Α	19	90.949	57.944	27.944	1.00 27.42	С
ATOM	157	N.	GLY	A	20	91.040	54.410	31.169	1.00 26.77	N
ATOM	158	CA	GLY		20	91.346	54.000	32.528	1.00 26.84	· C
ATOM	159	C	GLY		20	92.544	53.079	32.388	1.00 27.02	c
ATOM	160	Ō	GLY		20	93.130	53.018	31.314	1.00 26.32	o
ATOM	161	N	LEU		21	92.919	52.360	33.437	1.00 27.85	N
ATOM	162	CA	LEU		21	94.070	51.468	33.333	1.00 27.83	C
ATOM		C	LEU		21			32.500		C
	163					93.765	50.236		1.00 29.29	
ATOM	164	O GE	LEU		21	92.834	49.491	32.795	1.00 29.57	0
ATOM	165	CB	LEU		21	94.549	51.022	34.724	1.00 28.50	C
MOTA	166	CG	LEU		21	95.732	50.038	34.732	1.00 28.54	C
MOTA	167		LEU		21	96.928	50.654	34.003	1.00 27.17	C
MOTA	168		LEU		21	96.101	49.681	36.175	1.00 28.26	· C
MOTA	169	N	SER		22	94.552	50.032	31.449	1.00 30.33	N
ATOM	170	CA	SER		22	94.392	48.867	30.592	1.00 31.39	С
ATOM	171	C	SER		22	95.419	47.829	31.039	1.00 32.61	C
MOTA	172	. 0	SER	А	22	96.626	48.063	30.930	1.00 32.22	0
MOTA	173	CB	SER	A	22	94.650	49.233	29.131	1.00 31.24	, C
MOTA	174	OG	SER	Α	22	93.690	50.152	28.652	1.00 31.78	O.
MOTA	175	$N_{\cdot}$	THR	Α	23	94.941	46.693	31.547	1.00 33.62	N
ATOM	176	CA	THR	Α	23	95.821	45.620	32.007	1.00 34.86	C
ATOM	177	C	THR	Α	23	96.222	44.737	30.834	1.00 35.59	С
ATOM	178	0	THR	Α	23	95.573	44.757	29.786	1.00 35.63	. 0
MOTA	179	CB	THR	Α	23	95.132	44.727	33.059	1.00 35.00	С
MOTA	180	OG1	THR	A	23	93.945	44.160	32.493	1.00 36.07	0
MOTA	181	_CG2	THR	Α	23 .	94.766	45.533	34.295	1.00 35.01	С
ATOM	182	N	VAL	A	24	97.287	43.958	31.015	1.00 36.20	И
ATOM	183	CA	VAL		24	97.767	43.070	29.962	1.00 37.31	C
ATOM	184	С	VAL		24	96.717	42.041	29.553	1.00 38.42	Ç
MOTA	185	0	VAL		24	96.757	41.520	28.439	1.00 38.33	0
ATOM	186	СВ	VAL		24	99.053	42.308	30.388	1.00 37.05	C
ATOM	187		VAL		24	100.194	43.295	30.612	1.00 36.36	C
ATOM	188		VAL		24	98.786	41.485	31.642	1.00 36.49	. c
ATOM	189	N.	ASP		25	95.773	41.749	30.441	1.00 39.90	N
ATOM	190	CA	ASP		25	94.753	40.772	30.101	1.00 41.78	C
ATOM	191	C	ASP		25	93.581	41.335	29.298	1.00 41.86	C
ATOM	192	Ō	ASP		25	92.762	40.570	28.794	1.00 42.34	0
MOTA	193	СВ	ASP		25	94.251	40.050	31.362	1.00 43.81	· c
ATOM	194	CG	ASP		25	93.534	40.968	32.323	1.00 45.75	C
ATOM	195		ASP		25	92.406	41.397	32.011	1.00 47.52	0
ATOM	196		ASP		25	94.099	41.261	33'.400	1.00 47.32	
ATOM	197	N	CYS		26	93.485	42.656	29.151	1.00 41.52	. O
ATOM		CA								N
	198		CYS		26	92.374	43.173	28.363	1.00 41.49	C
ATOM	199	C	CYS		26	92.701	43.323	26.898	1.00 41.58	C
MOTA	200	0	CYS		26	93.229	44.343	26.456	1.00 41.10	0
ATOM	201	CB	CYS		26	91.854	44.522	28.856	1.00 40.64	C
ATOM	202	SG	CYS		26	90.147		28.259	1.00 40.94	, S
ATOM	203	N	ILE		27	92.379	42.281	26.151	1.00 42.19	. N
ATOM	204	CA	ILE		27	92.563	42.280	24.721	1.00 42.85	C
ATOM	205	C	ILE		27	91.140	42.075	24.226	1.00 43.07	. C
ATOM	206	0	ILE		27	90.327	41.450	24.911	1.00 42.66	. 0
MOTA	207	CB	ILE		27	93.491	41.125	24.265	1.00 43.47	C
MOTA	208		ILE		27	93.134	39.831	25.002	1.00 43.91	C
MOTA	209	CG2	ILE	A	27	94.940	41.501	24.523	1.00 43.28	С

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MOTA	210	CD1			27	94.064	38.662	24.686	1.00 4				С
MOTA	211	N	PRO		28	90.809	42.628	23.052	1.00 4				N
ATOM	212	CA	PRO'		28	89.476	42.516	22.456	1.00 4				Ç
ATOM	213	С	PRO		28	88.861	41.117	22.465	1.00 4				С
MOTA	214	0	PRO		28	87.685	40.956	22.797	1.00 4				0
ATOM	215	CB	PRO	A	28	89.696	43.049	21.044	1.00 4	4.02			С
MOTA	216	CG	PRO	A	28	90.692	44.142	21.277	1.00 4	3.69			С
MOTA	217	CD	PRO	Α	28	91.680	43.481	22.220	1.00 4	3.81			С
MOTA	218	N	SER	A	29.	89.654	40.109	22.116	1.00 4	3.37			N
MOTA	219	CA	SER	Α	29	89.152	38.739	22.065	1.00 4	3.09			С
ATOM	220	C	SER	Α	29	88.731	38.182	23.422	1.00 4	2.29			С
ATOM	221	0	SER	A	29	88.027	37.176	23.493	1.00 4	2.98			0
ATOM	222	CB	SER	A	29	90.192	37.810	21.414	1.00 4	3.86	•		С
ATOM	223	OG	SER	A	29	91.393	37.743	22.165	1.00 4	5.20			0
ATOM	224	N	ASN	Α	30	89.154	38.828	24.500	1.00 4	1.03			N
ATOM	225	CA	ASN		30	88.780	38.362	25.829	1.00 3	9.63			С
ATOM	226	С	ASN		30 .	87.608	39.158	26.410	1.00 3				C
ATOM	227	0	ASN		30	87.194	38.931	27.545	1.00 3				0
ATOM	228	CB	ASN		30	89.986	38.429	26.765	1.00 4				C
ATOM	229	CG	ASN		30	90.922	37.244	26.591	1.00 4				Ċ
ATOM	230		ASN		30 .	91.261	36.864	25.468	1.00 4				ō
ATOM	231		ASN		30	91.345	36.656	27.704	1.00 4				N
ATOM	232	N	VAL		31	87.072	40.088	25.627	1.00 3				N
ATOM	233	CA	VAL		31	85.948	40.894	26.087	1.00 3				C
		CA											C
ATOM	234		VAL		31	84.636	40.127	25.953	1.00 3				
ATOM	235	0	VAL		31	84.319	39.593	24.892	1.00 3				0
ATOM	236	CB	VAL		31	85.847	42.227	25.302	1.00 3				C
ATOM	237		VAL		31	84.590	42.989	25.715	1.00 3				C
MOTA	238		VAL		31	87.088	43.074	25.570	1.00 3				C
MOTA	239	N	ASN		32	83.887	40.075	27.047	1.00 3				N
ATOM	240	CA	ASN		32	82.604	39.383	27.088	1.00 3				С
MOTA	241	C	ASN		32	81.503	40.434	26.951	1.00 2				С
MOTA	242	0	ASN		32	81.363	41.307	27.804	1.00 2				0
MOTA	243	CB	ASN		32 .	82.474	38.633	28.421	1.00 3				С
MOTA	244	CG	ASN		32	81.174	37.862	28.542	1.00 3				С
MOTA	245	OD1	ASN	Α	32	80.279	37.978	27.705	1.00 3	1.47			0
ATOM	246	ND2	ASN	Α	32	81.062	37.068	29.604	1.00 3	2.67			N
ATOM	247	N	LEU	Α	33	80.728	40.343	25.875	1.00 2	8.85			N
MOTA	248	CA	LEU	A	33	79.647	41.290	25.591	1.00 2	8.13			C
ATOM	249	C	LEU	Α	33	78.259	40.780	25.983	1.00 2	7.84			С
ATOM	250	0	LEU	Α	33	77.240	41.298	25.524	1:00 2	8.25			0
MOTA	251	CB	LEU	Α	33	79.662	41.637	24.101	1.00 2	7:87	•		С
MOTA	252	CG	LEU	Α	33	80.228	42.982	23.621	1.00 2	8.18			С
MOTA	253	CD1	LEU	Α	33	81.299	43.515	24.546	1.00 2	7.71			С
ATOM	254	CD2	LEU	A	33	80.757	42.799	22.215	1.00 2	7.10			С
MOTA	255	N	SER		34	78.223	39.762	26.828	1.00 2	7.39			N
ATOM	256	CA	SER		34	76.963	39.183	27.291	1.00 2	7.16			С
ATOM	257	C	SER		34	76.204	40.218	28.129	1.00 2				С
ATOM	258	0	SER		34	76.814	41.063	28.774	1.00 2		-		0
ATOM	259	CB	SER		34	77.263	37.930	28.124	1.00 2				Ċ
ATOM	260	OG	SER		34	76.102	37.434	28.756	1.00 3				ō
ATOM	261	N	THR		35	74.877	40.157	28.124	1.00 2			,	N
	262	CA	THR		35	74.095	41.125	28.885	1.00 2				C
ATOM	263	C	THR		35	72.687	40.592	29.158	1.00 2				C
ATOM	264	0	THR		35	72.115	39.865	28.344	1.00 2				0
ATOM	265	CB	THR		35	74.021	42.485	28.121	1.00 2				C
ATOM	266				35		43.549	29.040					0
AIOM	200	OGI	THR	A	22	73.744	43.343	49.040	1.00 2	۵.∠٥			U

ATOM	267	CG2	THR	Α	35	72.931	42.456	27.070	1.00 24.69		С
ATOM	268	N	PRO	A	36	72.109	40.948	30.314	1.00 24.52		N
ATOM	269	CA	PRO	A ·	36	70.761	40.485	30.665	1.00 24.57		C
MOTA	270	С	PRO	A	36	69.651	41.167	29.867	1.00 25.00		C
MOTA	271	0	PRO	A	36	69.697	42.375	29.631	1.00 25.19		0
MOTA	272	CB	PRO	Α	36	70.672	40.797	32.155	1.00 24.46		C
ATOM	273	CG	PRO	Α	36 ·	71.479	42.072	32.264	1.00 24.23		C
ATOM	274	CD	PRO	A	36	72.684	41.786	31.383	1.00 24.01		C
ATOM	275	N	LEU	Α	37	68.651	40.393	29.456	1.00 24.96		N
ATOM	276	CA	LEU	Α	37	67.535	40.946	28.705	1.00 25.21		C
ATOM	277	С	LEU	Α	37	66.308	41.179	29.593	1.00 25.43		C
MOTA	278	0	LEU	A	37	65.599	42.175	29.426	1.00 25.20		0
MOTA	279	CB	LEU	A`	37	67.156	40.017	27.546	1.00 24.90		С
MOTA	280	CG	LEU	Α	37	66.049	40.506	26.599	1.00 25.00		С
MOTA	281	CD1	LEU	Α.	37	66.593	41.629	25.709	1.00 24.59		C
MOTA	282	CD2	LEU	Α	37	65.550	39.351	25.729	1.00 24.58		C
MOTA	283	N	VAL	Α	38	66.061	40.274	30.539	1.00 25.54		N
MOTA	284	CA	VAL	A	38	64.896	40.397	31.415	1.00 25.63		С
MOTA	285	С	VAL	A	38	65.241	40.442	32.904	1.00 26.35		C
MOTA	286	0	VAL	A	38	66.268	39.919	33.335	1.00 26.41		0
MOTA	287	CB	VAL	Α	38	63.885	39.262	31.136	1.00 25.83		C
MOTA	288	CG1	VAL	A	38	63.410	39.357	29.679	1.00 25.31		C
MOTA	289	CG2	VAL	A	38	64.523	37.895	31.398	1.00 24.98		С
MOTA	290	N	LYS	Α	39	64.368	41.074	33.682	1.00 26.62		N
MOTA	291	CA	LYS	A	39	64.588	41.251	35.113	1.00 27.40		С
MOTA	292	C	LYS	A	39	64.768	39.986	35.943	1.00 27.98		С
MOTA	293	0	LYS	A	39	64.220	38.926	35.625	1.00 28.34		0
MOTA	294	CB	LYS	Α	39	63.453	42.085	35.722	1.00 27.32		С
MOTA	295	CG	LYS	A	39	62.098	41.400	35.710	1.00 27.27		С
MOTA	296	CD	LYS	A	39	61.075	42.203	36.491	1.00 27.48		С
MOTA	297	CE	LYS	A	39	59.703	41.538	36.465	1.00 27.05		С
MOTA	298	NZ	LYS	A	39	58.735	42.262	37.335	1.00 26.75		N
MOTA	299	N	PHE	A	40	65.539	40.133	37.017	1.00 28.20		N
MOTA	300	CA	PHE	Α	40	65.828	39.057	37.958	1.00 29.34		C
MOTA	301	C	PHE	Α	40	66.082	39.682	39.337	1.00 30.13		С
MOTA	302	0	PHE	A	40 .	66.226	40.899	39.447	1.00 30.16		0
MOTA	303	CB	PHE	Α	40	67.058	38.258	37.501	1.00 28.35		С
MOTA	304	CG	PHE	A	40	68,264	39.110	37.197	1.00 27.78		С
MOTA	305	CD1	PHE	A	40	68.448	39.650	35.924	1.00 26.96		C.
MOTA	306	CD2	PHE	Α.	40	69.209	39.379	38.183	1.00 27.28		C
MOTA	307	CE1	PHE	Α	40	69.553	40.442	35.635	1.00 26.45		Ċ
MOTA	308	CE2	PHE	Α	40	70.325	40.174	37.907	1.00 27.06		С
MOTA	309	CZ	PHE	Α	40	70.497	40.706	36.628	1.00 27.14		С
MOTA	310	N	GLN	Α	41	66.130	38.851	40.379	1.00 31.29		N
MOTA	311	CA	GLN	Α	41	66.358	39.317	41.754	1.00 32.59		C
MOTA	312	С	GLN	Α	41	67.851	39.354	42.054	1.00 32.23		C
MOTA	313	0	GLN	A	41	68.637	38.714	41.362	1.00 31.49		0
MOTA	314	CB	GLN	Α	41	65.698	38.365	42.759	1.00 34.28		С
ATOM	315	CG	GLN	Α	41	64.249	38.045	42.486	1.00 37.74		С
ATOM '	316	CD	GLN	Α	41	63.310	39.092	43.041	1.00.40.33		С
MOTA	317	OE1	GLN	Α	41	63.397	40.277	42.694	1.00 41.23		0
MOTA	318	NE2	GLN	A	41	62.397	38.662	43.916	1.00 41.92		N
MOTA	319	N	LYS	A	42	68.245	40.084	43.095	1.00 32.61		N
MOTA	320	CA	LYS		42	69.659	40.152	43.442	1.00 33.23	•	C
ATOM	321	C	LYS		42 '	70.235	38.768	43.716	1.00.33.05		C
ATOM	322	0	LYS		42	69.609	37.943	44.384	1.00 32.65		0
ATOM	323	CB	LYS		42	69.898	41.024	44.672	1.00 34.37		C

7 IIIOM	224	00	TVC	70	4.0	71.380	41.106	45.002	1.00 36.49		С
MOTA	324	CG	LYS		42						
ATOM	325	CD	LYS		42	71.712	42.108	46.093	1.00 38.56		C
MOTA	326	CE	LYS		42	71.361	41.595	47.463	1.00 38.86		C
MOTA	327	NZ	LYS	A	42	71.973	42.474	48.502	1.00 40.12		N
ATOM	328	N	GLY	Α	43	71.432	38.518	43.198	1.00 32.94		N
ATOM	329	CA	GLY	Α	43	72.064	37.231	43.414	1.00 32.98		·C
ATOM	330	С	GLY	Α	43	71.847	36.234	42.297	1.00 32.97		С
ATOM	331	0	GLY		43	72.611	35.279	42.170	1.00 32.75		0
ATOM	332	N	GLN		44	70.815	36.430	41.483	1.00 33.23	\$	N
									1.00 33.23		C
ATOM	333	CA	GLN		44	70.580	35.498	40.388			
ATOM	334	,C	GLN		44	70.996	36.029	39.023	1.00 33.69		C
ATOM	335	0	GLN		44	71.505	37.139	38.906	1.00 33.63		0
ATOM	336	CB	GLN	Α	44	69.113	35.039	40.362	1.00 34.55		С
MOTA	337	CG	GLN	Α	44	68.093	36.090	40.695	1.00 35.61		С
ATOM	338	CD	GLN	Α	44	66.677	35.538	40.781	1.00 35.93		С
ATOM	339	OE1	GLN	Α	44	66.382	34.665	41.599	1.00 37.13		0
MOTA	340	NE2				65.793	36.051	39.938	1.00 35.37		N
ATOM	341	N	GLN		45	70.803	35.204	37.999	1.00 33.77		N
	342	CA	GLN		45	71.135	35.560	36.623	1.00 33.60		C
ATOM	343	C ·			45	69.832	35.752	35.874	1.00 33.34		C
ATOM	344	0	GLN		45	68.794	35.245	36.287	1.00 31.56		0
ATOM	345	СВ	GLN		45	71.921	34.432	35.938	1.00 35.04		C
ATOM	346	CG	GLN		45	73.297	34.165	36.516	1.00 37.78		С
MOTA	347	CD	GLN		45	74.285	35.267	36.191	1.00 39.44		C
ATOM	348	OE1	GLN	A	45	74.613	35.497	35.022	1.00 40.59	•	0
MOTA	349	NE2	GLN	Α	45	74.767	35.959	37.225	1.00 39.68		N
ATOM	350	N	SER	Α	46	69.889	36.483	34.771	1.00 31.43		N
ATOM	351	CA	SER		46	68.701	36.703	33.969	1.00 31.01		С
ATOM	352	C	SER		46	68.396	35.419	33.211	1.00 30.99		С
ATOM	353	0	SER		46	69.312	34.730	32.766	1.00 31.11		0
ATOM	354	CB	SER		46	68.931	37.833	32.964	1.00 30.11		C
ATOM	355				46			32.219	1.00 28.77		0
		OG	SER			67.752	38.074				
ATOM	356	N	GLU		47	67.113	35.100	33.068	1.00 31.10		N
ATOM	357	CA	GLU		47	66.708	33.905	32.337	1.00 31.53		C
ATOM	358	C	GLU		47	67.119	34.002	30.877	1.00 31.11	,	Ç
MOTA	359	0	GLU		47	67.311	32.985	30.215	1.00 31.30		0
MOTA	360	CB	GLU	A	47	65.198	33.710	32.427	1.00 32.16		С
ATOM	361	CG	${\tt GLU}$	Α	47	64.717	33.337	33.814	1.00 34.70		С
ATOM	362	CD	GLU	A	47 ·	63.211	33.402	33.933	1.00 36.22		С
ATOM	363	OE1	GLU	Α	47	62.524	32.650	33.208	1.00 37.59		0
ATOM	364	OE2			47	62.715	34.211	34.747	1.00 37.82		0
ATOM	365	N	ILE	Α	48	67.233	35.226	30.367	1.00 30.49		N
ATOM	366	CA	ILE		48	67.643	35.431	28.981	1.00 29.71		C
ATOM	367 ⁻	C	ILE		48	68.791	36.432	28.911	1.00 29.44		C
									1.00 29.08		0
ATOM	368	0	ILE		48	68.670	37.575	29.356			
ATOM	369	CB	ILE		48	66.488	35.962	28.099	1.00 30.08		C
MOTA	370		ILE		48	65.281	35.021	28.171	1.00 30.16		С
MOTA	371		ILE		48	66.967	36.091	26.653	1.00 29.55		С
MOTA	372	CD1	ILE	А	48	64.082	35.489	27.348	1.00 29.84	. ,	С
MOTA	373	N	ASN	А	49	69.905	35.988	28.347	1.00 28.86		N
MOTA	3.74	CA	ASN	Α	49	71.085	36.820	28.198	1.00 29.07		С
MOTA	375	С	ASN		49	71.483	36.882	26.730	1.00 28.95		С
ATOM	376	0	ASN		49	71.609	35.852	26.067	1.00 29.13		0
ATOM	377	СВ	ASN		49	72.245	36.245	29.021	1.00 28.75		C
ATOM	378	CG	ASN		49	72.023	36.385	30.515	1.00 28.90		C
MOTA	379		ASN		49	72.023	37.459	31.084	1.00 28.55		σ
MOTA	380				49			31.155	1.00 29.52		И
WI ON	300	אחצ	ASN	A	せり	71.609	35.302	31.133	1.00 49.34		₹A

MOTA	381	N	LEU	A	50	71.658	38.094	26.220	1.00 28.25		N
MOTA	382	CA	LEU	Α	50	72.071	38.273	24.834	1.00 27.70		C
MOTA	383	C	LEU	A	50	73.568	37.994	24.791	1.00 27.62	•	С
MOTA	384	0	LEU	A	50	74.252	38.178	25.793	1.00 27.10	•	0
MOTA	385	CB	LEU	A	50	71.814	39.718	24.389	1.00 26.87		С
MOTA	386	CG	LEU	A	50	70.381	40.241	24.527	1.00 27.52		C
MOTA	387	CD1	LEU	A	50	70.339	41.740	24.227	1.00 27.19		C
MOTA	388	CD2	LEU	A	50	69.467	39.465	23.588	1.00 27.05		C
ATOM	389	N	LYS		51 .	74.073	37.541	23.646	1.00 28.04		N
MOTA	390	CA	LYS		51	75.507	37.286	23.493	1.00 28.80		C
ATOM	391	C	LYS		51	76.182	38.622	23.166	1.00 27.80		C
ATOM	392	0	LYS		51	77.351	38.834	23.481	1.00 28.10		0
ATOM	393	CB	LYS		51	75.772	36.277	22.364	1.00 30.63		C
ATOM	394	CG	LYS		51	76.038	34.848	22.827	1.00 32.96		C
MOTA	395	CD	LYS		51	74.829	34.217	23.460	1.00 34.61		C
MOTA	396	CE	LYS		51	75.131	32.788	23.913	1.00 35.94		. C
MOTA	397	NZ	LYS		51	75.513	31.887	22.788	1.00 36.84		N
MOTA	398	N	ILE		52	75.431	39.508	22.518	1.00 26.90		N
MOTA	399	CA	ILE		52	75.899	40.848	22.177	1.00 26.16		C
ATOM	400	C	ILE		52	74.759	41.798	22.556	1.00 26.14		C
MOTA	401	0	ILE		52	73.583	41.452	22.430	1.00 26.42		0
ATOM	402	CB	ILE		52	76.247	40.989	20.671	1.00 25.90		C
ATOM	403	CG1	ILE		52	75.041	40.634	19.803	1.00 25.37		C
MOTA	404	CG2	ILE		52	77.443	40.086	20.329	1.00 25.95		C
MOTA	405	CD1	ILE		52	75.244	40.975	18.331	1.00 24.51		C
ATOM	406	N	PRO		53	75.093	43.011	23.016	1.00 25.79		N
ATOM	407 408	CA C	PRO		53	74.090	43.999	23.431	1.00 25.66		C
ATOM ATOM		0 -	PRO PRO		53 53	73.334	44.765	22.345	1.00 25.90		C
ATOM	.409 410	CB	PRO		53	73.041	45.947	22.521	1.00 26.17		. 0
ATOM	411	CG	PRO		53	74.900 76.207	44.929 44.999	24.319 23.568	1.00 24.87 1.00 25.16		C C
ATOM	412	CD	PRO		53	76.459	43.553	23.167	1.00 25.10		C
ATOM	413	N	LEU		54	73.002	44.101	21.241	1.00 25.11		N
MOTA	414	CA	LEU		54	72.285	44.767	20.157	1.00 25.81		C
MOTA	415	C	LEU		54	70.975	44.072	19.799	1.00 26.02		, C
ATOM	416	Ō	LEU		54	70.931	42.847	19.653	1.00 26.13		. 0
MOTA	417	СВ	LEU		54	73.160	44.839	18.897	1.00 25.47		C
ATOM	418	CG	LEU		54	74.556	45.459	19.009	1.00 26.34		C
ATOM	419	CD1	LEU		54 ·	75.216	45.494	17.627	1.00 26.06		C
ATOM	420	CD2	LEU	A	54	74.458	46.863	19.591	1.00 26.01		C
MOTA	421	N	VAL	A	55	69.911	44.858	19.668	1.00 25.53		N
MOTA	422	CA	VAL	A	55 .	68.614	44.325	19.277	1.00 25.73		С
MOTA	423	C	VAL	A	55	68.078	45.236	18.172	1.00 26.28		С
MOTA	424	0	VAL	Α	55	68.287	46.455	18.207	1.00 26.42		0
MOTA	425	CB	VAL	A	55	67.612	44.265	20.477	1.00 25.52		C
ATOM	426	CG1	VAL	Α	55	68.262	43.550	21.654	1.00 24.72		C
ATOM	427	CG2	VAL	A	<b>5</b> 5	67.139	45.656	20.868	1.00 24.62		C
ATOM	<b>1.428</b>	N	SER	A	56	67.418	44.652	17.174	1.00 26.19		N
ATOM	429	CA	SER	A	56	66.884	45.447	16.073	1.00 25.97		C
ATOM	430	C.	SER		56	65.508	46.017	16.417	1.00 25.83		C
ATOM	431	0	SER		56	64.700	45.373	17.089	1.00 25.99		0
ATOM	432	CB	SER		56	66.831	44.610	14.788	1.00 25.77		С
ATOM	433	OG	SER		56	66.050	43.446	14.965	1.00 26.05		0
ATOM	434	N	ALA		57	65.264	47.238	15.957	1.00 25.89		N
ATOM	435	CA	ALA		57	64.024	47.966	16.218	1.00 26.47		C
ATOM	436	C	ALA		57	62.721	47.300	15.756	1.00 27.16		C
ATOM	437	0	ALA	A	57	62.692	46.554	14.779	1.00 27.22		0

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MOTA	438	CB	ALA		57	64.133	49.358	15.619	1.00 25.6		
MOTA	439	N	ILE	Α	58	61.643	47.594	16.478	1.00 27.6		
· MOTA	440	CA	ILE	Α	58	60.316	47.056	16.184	1.00 28.4	1 (C	:
ATOM	441	С	ILE	Α	58	59.737	47.863	15.021	1.00 28.8	6 C	1
ATOM	442	0	ILE	Α	58	58.795	48.644	15.194	1.00 29.0	4 0	)
ATOM	443	CB	ILE		58	59.388	47.204	17.414	1.00 27.8	6 C	•
ATOM	444	CG1	ILE		58	60.156	46.808	18.683	1.00 27.4		
									1.00 27.8		
ATOM	445	CG2	ILE		58	58.145	46.335	17.239			
ATOM	446	CD1			58	59.338	46.846	19.959	1.00 26.0		
ATOM	447	N	MET	Α	59	60.304	47.659	13.836	1.00 29.0		
ATOM	448	CA	MET	Α	59	59.896	48.407	12.652	1.00 29.9	·3 C	•
ATOM	449	С	MET	Α	59	59.747	47.546	11.400	1.00 30.4	.1 C	2
MOTA	450	0	MET	Α	59	60.510	46.605	11.185	1.00 29.9	6 C	)
ATOM	451	CB	MET		59	60.922	49.507	12.379	1.00 29.6		
ATOM	452	CG	MET		59	61.172	50.439	13.556	1.00 29.0		
									1.00 29.3		
ATOM	453	SD	MET		59 .	62.564	51.543	13.248			
ATOM	454	CE	MET		59	61.850	52.630	12.008	1.00 28.2		
ATOM	455	N	GLN		60	58.766	47.901	10.575	1.00 31.5		
MOTA	456	CA	GLN	A	60	58.476	47.186	9331	1.00 32.5		
ATOM	457	C ·	GLN	A	60	59.685	47.152	8.411	1.00 32.7	'6 C	1
	458	0	GLN	A	60	59.904	46.173	7.707	1.00 32.7	'0 ° C	)
MOTA	459	CB	GLN		60	57.334	47.862	8.565	1.00 32.8		
ATOM	460	CG	GLN		60	56.084	48.176	9.362	1.00 34.0		
			GLN				48.821	8.497	1.00 34.7		
MOTA	461	CD			60	55.010					
MOTA	462	OE1			60	55.313	49.611	7.603	1.00 35.7		
MOTA	463	NE2	GLN	A	60	53.749	48.497	8.767	1.00 35.2		
MOTA	464	N	SER	A	61	60.463	48.232	8.418	1.00 33.3		
MOTA	465	CA	SER	Α	61	61.629	48.334	7.552	1.00 33.3	0 C	-
MOTA	466	С	SER	Α	61	62.931	47.752	8.099	1.00 33.2	:0 C	3
ATOM	467	0	SER	A·	61	63.988	47.933	7.492	1.00 33.6	51 0	)
ATOM	468	CB	SER		61	61.853	49.799	7.143	1.00 33.4		7
ATOM	469	OG	SER		61	62.047	50.635	8.271	1.00 35.0		
		N.				62.875	47.052	9.227	1.00 32.7		
ATOM	470		VAL		62 .						
MOTA	471	CA	VAL		62	64.101	46.475	9.764	1.00 32.5		
MOTA	472	C	VAL		62	63.999	45.079	10.358	1.00 32.6		
ATOM	473	0	VAL	Α	62	64.800	44.213	10.026	1.00 33.5		
MOTA	474	CB	VAL	A	62	64.789	47.432	10.810	1.00 32.4		
ATOM	475	CG1	VAL	Α	62	63.860	48.545	11.206	1.00 32.3	31 (	7
MOTA	476	CG2	VAL	Α	62	65.245	46.655	12.041	1.00 31.5	54 (	2
	.477	N	SER	Α.	63	63.017	44.838	11.215	1.00 33.0	)4 N	Ţ
ATOM	478	CA	SER		63	62.924	43.531	11.845	1.00 32.7		
ATOM	479	C	SER		63	61.986	42.510	11.214	1.00 33.0		
					•						
ATOM	480	0	SER		63	60.871	42.283	11.692	1.00 32.0		
MOTA	481	ĊВ	SER		63	62.600	43.700	13.331	1.00 32.7		
MOTA	482	OG	SER		63	63.666	44.356	14.005	1.00 31.7		
ATOM	483	N	GLY	A	64	62.467	41.894	10.138	1.00 33.4		
ATOM .	.484	CA	GLY	Α	64	61.717	40.857	9.454	1.00 33.9	96 (	3
MOTA	485	C.	GLY	Α	64	62.338	39.518	9.829	1.00 34.6	58 C	2
ATOM	486	0	GLY	A	64	63.160	39.455	10.749	1.00 33.8	36 0	)
ATOM	487	N	GLU		65	61.961	38.453	9.123	1.00 35.4		
ATOM	488	CA	GLU		65	62.482	37.113	9.394	1.00 36.6		
		C	GLU		65	63.987	36.993	9.207	1.00 36.6		
ATOM	489										
ATOM	490	0	GLU		65	64.694	36.532	10.101	1.00 36.5		
ATOM	491	CB	GLU		65	61.809	36.077	8.489	1.00 38.3		
MOTA	492	CG	GLU		65	60.441	35.608	8.946	1.00 41.0		
ATOM	493	CD	GLU	Α	65	59.808	34.623	7.964	1.00 42.5		2
MOTA	494	OE1	GLU	A	65	60.483	33.631	7.595	1.00 43.4	ł3 (	)

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MOTA	495	OE2	GLU	A	65	58.639	34.844	7.568	1.00 42.9	0	0
MOTA	496	N	LYS	Α	66	64.470	37.386	8.033	1.00 36.5	0	N
MOTA	497	CA	LYS	A	66	65.891	37.293	7.734	1.00 36.6	7	C
ATOM	498	C	LYS	A	66 .	66.729	38.082	8.734	1.00 35.7	0	C
ATOM	499	0	LYS	A	66	67.803	37.639	9.137	1.00 35.1	0	0
ATOM	500	ĊB	LYS	A	66	66.164	37.775	6.304	1.00 37.8	3.	С
MOTA	501	CG	LYS	A	66	65.512	36.899	5.242	1.00 40.0	2	С
MOTA	502	CD	LYS	A	66	65.935	37.299	3.828	1.00 42.3	3	С
MOTA	503	CE	LYS		66	65.202	36.465	2.776	1.00 43.2	1	С
ATOM	504	NZ	LYS		66	65.582	36.849	1.381	1.00 44.5	7	N
MOTA	505	N	MET	Α	67	66.231	39.247	9.134	1.00 34.6	1	N
MOTA	506	CA	MET		67	66.938	40.068	10.105	1.00 33.5	5	С
MOTA	507	С	MET		67	67.023	39.306	11.427	1.00 32.8		С
ATOM	508	0	MET		67	68.104	39.148	11.995	1.00 32.2		0
ATOM	509	СВ	MET		67	66.204	41.394	10.322	1.00 33.3		C
ATOM	510	CG	MET		67	66.868	42.316	11.338	1.00 32.8		C
ATOM	511	SD	MET		67	68.526	42.816	10.844	1.00 32.4		s
ATOM	512	CE	MET		67	68.141	43.942	9.476	1.00 31.5		C
ATOM	513	И	ALA		68	65.877	38.825	11.899	1.00 31.9		N
ATOM	514	CA	ALA		68	65.811	38.093	13.156	1.00 31.6		C
ATOM	515	C ·	ALA		68	66.789	36.928	13.130	1.00 31.0		Ç
MOTA	516	0	ALA		68	67.459	36.686	14.190	1.00 31.7		0
ATOM	517	CB	ALA		68	64.389	37.592	13.394	1.00 31.7		C
ATOM	518	N							1.00 31.3		
ATOM			ILE		69	66.866	36.203	12.073			N C
	519	CA	ILE		69	67.766	35.061	11.969	1.00 31.1		
ATOM	520	C	ILE		69	69.226	35.511	11.942	1.00 30.5		C
	521	0	ILE		69	70.059	34.992	12.686	1.00 30.9		0
ATOM	522		ILE		69	67.452	34.234	10.691	1.00 31.7		C
ATOM	523	CG1			69	66.083	33.563	10.836	1.00 32.1		C
ATOM	524	CG2	ILE		69	68.529	33.184	10.459	1.00 32.0		C
ATOM	525	CD1			69	65.529	33.009	9.536	1.00 32.4		C
ATOM	526	N	ALA		70	69.526	36.484	11.088	1.00 29.8		N
MOTA	527	CA	ALA		70	70.882	36.998	10.953	1.00 29.2		С
MOTA	528	C	ALA		70	71.425	37.592	12.249	1.00 28.8		C
MOTA	529	0	ALA		70	72.589	37.391	12.583	1.00 28.3		0
MOTA	530	CB	ALA		70	70.932	38.041	9.847	1.00 29.1	.7 .	C
ATOM	531 .	N	LEU		71	70.585	38.324	12.979	1.00 28.7		N
MOTA	532	CA	LEU		71	71.027	38.937	14.224	1.00 28.3		C
ATOM	533	С	LEU		71	71.187	37.890	15.316	1.00 28.4		С
MOTA	534	0	LEU		71	72.158	37.913	16.064	1.00 27.5		0
MOTA	535	CB	LEU	A	71	70.044	40.021		1.00 27.9		C
ATOM	536	CG	LEU	А	71	70.409	40.792	15.945	1.00 27.6	5	C
MOTA	537		LEU		71	71.861	41.254	15.890	1.00 26.8	3	, C
MOTA	538	CD2	LEU	Α	71	69.476	41.990	16.092	1.00 27.3	4	C
MOTA	539 -	N	ALA	Α	72	70.235	36.967	15.398	1.00 29.1	.1	N
ATOM	540	CA	ALA	A	72	70.302	35.911	16.400	1.00 30.0	5	С
ATOM	541	C	ALA	А	72	71.587	35.109	16.211	1.00 30.7	3	C
ATOM	542	0	ALA	A	72 .	72.212	34.688	17.187	1.00 30.2	2	0
MOTA	543	CB	ALA	Α	72	69.081	34.992	16.288	1.00 29.9	9	C
MOTA	544	N	ARG	Α	73	71.980	34.900	14.955	1.00 31.5	1	N
MOTA	545	CA	ARG	Α	73	73.203	34.152	14.659	1.00 32.6	0	С
MOTA	546	C	ARG		73	74.432	34.827	15.253	1.00 32.5	9	С
ATOM	547	0	ARG		73	75.402	34.161	15.602	1.00 32.7		0
MOTA	548	CB	ARG		73	73.392	34.000	13.147	1.00 33.5		С
MOTA	549	CG	ARG		73	72.540	32.910	12.528	1.00 35.3		. C
MOTA	550	CD	ARG		73	72.697	32.866	11.022	1.00 36.9		С
ATOM	551	NE	ARG		73	71.978	31.732	10.448	1.00 39.1		N
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MOTA	552	CZ	ARG	A	73	71.740	31.572	9.149	1.00	39.97		С
MOTA	553	NH1	ARG	A	73	72.161	32.476	8.274	1.00	39.65		N
MOTA	554	NH2	ARG	A	73	71.075	30.505	8.726	1.00	40.71		N
ATOM	555	N	GLU	A	74	74.384	36.151	15.368	1.00	32.40		N
ATOM	556	CA	GLU	A	74	75.498	36.908	15.920	1.00	32.28		С
MOTA	557	C	GLÜ	A	74	75.397	37.091	17.430	1.00	31.45		С
MOTA	558	0	GLU	A	74	76.299	37.642	18.047	1.00	31.66		0
MOTA	559	CB	GLU	A	74	75.595	38.274	15.235	1.00	33.47		С
ATOM	560	CG-	GLU	А	74	75.967	38.197	13.759	1.00	35.41		C
ATOM	561	CD	GLU	А	74	77.306	37.510	13.524	1.00	37.04		С
MOTA	562	OE1	GLU	A	74	78.337	38.018	14.017	1.00	37.82		0
MOTA	563	OE2	GLU	Α	74	77.325	36.458	12.846	1.00	38.54		0
MOTA	564	N	$\operatorname{GLY}$	Α	75	74.295	36.646	18.026	1.00	30.81		N
MOTA	565	CA	GLY	Α	75	74.152	36.774	19.467	1.00	30.19		C
ATOM	566	С	GLY	Α	75	73.133	37.780	19.966	1.00	29.59		С
ATOM	567	0	GLY	Α	75	72.909	37.888	21.176	1.00	28.90		0
MOTA	568	N	GLY	Α	76	72.524	38.522	19.044	1.00	29.15		N
MOTA	569	CA	GLY	Α	76	71.526	39.504	19.427	1.00	28.52		С
MOTA	570	С	GLY	Α	76	70.124	38.968	19.194	1.00	28.42		С
ATOM	571	0	GLY	Α	76	69.949	37.769	18.970	1.00	28.19		0
ATOM	572	N	ILE	A	77	69.124	39.846	19.250	1.00	27.85	•	N
ATOM	573	CA	ILE	A	77	67.744	39.435	19.026	1.00	27.34		С
ATOM	574	C	ILE	Α	77	66.963	40.538	18.315	1.00	27.73		С
MOTA	575	0	ILE	Α	77	67.228	41.730	18.507	1.00	27.71		0
MOTA	576	CB	ILE	A	77	67.043	39.089	20.363	1.00	26.95		С
ATOM	577	CG1	ILE	Α	77	65.811	38.217	20.097	1.00	26.86		С
MOTA	578	CG2	ILE	A	77	66.642	40.370	21.099	1.00	26.54		С
ATOM	579	CD1	ILE	Α	77	65.128	37.709	21.362	1.00	25.58		С
MOTA	580	N	SER	Α	78	66.010	40.135	17.481	1.00	27.61		N
MOTA	581	CA	SER	А	78	65.176	41.083	16.752	1.00	27.42		С
ATOM	582	C	SER	A	78	63.763	41.054	17.313	1.00	27.91		C
ATOM	583	0	SER	A	78	63.317	40.045	17.858	1.00	27.91		0
MOTA	584	CB	SER	A	78 .	65.104	40.721	15.264	1.00	26.86		C
MOTA	585	OG	SER	A	78	66.353	40.859	14.618	1.00	26.59		0
MOTA	586	N	PHE	Α	79	63.056	42.166	17.180	1.00	28.37		N
MOTA	587	CA	PHE	A	79	61.681	42.228	17.634	1.00	28.70		С
ATOM	588	C	PHE	Α	79	60.796	42.394	16.403	1.00	29.22		С
MOTA	589	0	PHE	Α	79	60.599	43.505	15.920	1.00	29.28		0
MOTA	590	CB	PHE	Α	79	61.489	43.389	18.620	1.00	28.26		C
MOTA	591	CG	PHE	A	79	62.076	43.121	19.980	1.00	28.13		C
MOTA	592	CD1	PHE	A	79	63.421	43.363	20.234	1.00	28.01	•	C
ATOM	593	CD2	PHE	A	79	61.291	42.574	20.995	1.00	28.23		C
MOTA	594	CE1	PHE	Α	79	63.981	43.063	21.479	1.00	28.23		C
MOTA	595	CE2	PHE	Α	79	61.840	42.270	22.244	1.00	27.87		C
MOTA	596	CZ	PHE	A	79	63.185	42.514	22.485	1.00	27.96		C
MOTA	597	N	ILE	Α	80	60.286	41.279	15.880	1.00	30.20		N
ATOM	598	CA	ILE	Α	80	59.426	41.316	14.697	1.00	30.73		C
ATOM	599	C	ILE	А	80	58.372	42.393	14.884	1.00	31.00		C
MOTA	600	0	ILE	Α	80	57.661	42.407	15.892	1.00	30.84		0
MOTA	601	CB	ILE	A	80	58.730	39.948	14.441	1.00	31.03		С
ATOM	602	CG1	ILE	Α	80	59.673	39.001	13.696	1.00	31.69		С
ATOM	603	CG2	ILE	Α	80	57.508	40.137	13.549	1.00	30.82		С
MOTA	604	CD1	ILE	A	80	60.976	38.770	14.361	1.00	32.86		С
MOTA	605	N	PHE	Α	81	58.277	43.299	13.914	1.00	31.46		N
MOTA	606	CA	PHE	A	81	57.318	44.387	14.010	1.00	32.33		С
MOTA	607	C	PHE	A	81	55.884	43.903	14.193	1.00	32.76		С
ATOM	608	Ó	PHE	A	81	55.464	42.908	13.595	1.00	32.74		0

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MOTA	609	СВ	PHE	Α	81	57.417	45.316	12.788	1.00 32.73		С
ATOM	610	CG	PHE	A	81	57.167	44.635	11.470	1.00 33.07		С
MOTA	611	CD1	PHE	Α	81	58.155	43.859	10.872	1.00 33.23		С
ATOM	612	CD2	PHE	Α	81	55.949	44.796	10.812	1.00 33.18		C
MOTA	613	CE1	PHE	Α	81	57.937	43.251	9.629	1.00 33.42		С
ATOM	614	CE2	PHE	Α	81	55.717	44.194	9.571	1.00 33.24		С
ATOM	615	CZ	PHE	А	81	56.716	43.420	8.979	1.00 33.26		С
ATOM	616	N	GLY	А	82	55.143	44.615	15.035	1.00 33.07		N
MOTA	617	CA	GLY	Α	82	53.763	44.260	15.303	1.00 34.00		C
MOTA	618	C	GLY	А	82	52.780	45.069	14.481	1.00 34.67		С
MOTA	619	0	GLY	Α	82	51.567	44.884	14.600	1.00 34.70		0
MOTA	620	N	SER	Α	83	53.300	45.971	13.651	1.00 35.05		N
ATOM	621	CA	SER	A	83	52.459	46.795	12.791	1.00 35.41	•	C
MOTA	622	C	SER	A	83	52.095	45.999	11.538	1.00 36.15		С
MOTA	623	0	SER	Α	83	52.438	46.367	10.411	1.00 36.11		0
MOTA	624	CB	SER	Α	83	53.185	48.085	12.409	1.00 35.00		C
ATOM	625	OG	SER	А	83	54.407	47.807	11.755	1.00 34.80		0
ATOM	626	N	${\tt GLN}$	Α	84	51.411	44.884	11.766	1.00 36.71		N
ATOM	627	CA	GLN	Α	84	50.952	43.993	10.714	1.00 37.15		С
ATOM	628	C	${\tt GLN}$	Α	84	49.907	43.107	11.386	1.00 37.55		C
ATOM	629	0	GLN	Α	84	49.734	43.173	12.605	1.00 37.38		Ó
MOTA	630	CB	GLN	A	84	52.115	43.157	10.165	1.00 37.55		С
ATOM	631	· CG	GLN	Α	84	52.783	42.238	11.179	1.00 37.88		С
ATOM	632	CD	GLN	A	84	53.907	41.426	10.569	1.00 38.47		С
ATOM	633	OE1	GLN	A	84	53.730	40.791	9.530	1.00 39.45		0
ATOM	634	NE2	GLN	Α	84	55.072	41.435	11.214	1.00 38.16		N
MOTA	635	N	SER	Α	85	49.208	42.286	10.610	1.00 37.98		N
ATOM	636	CA	SER	Α	85	48.177	41.427	11.183	1.00 38.63		С
ATOM	637	С	SER	A	85	48.755	40.456	12.205	1.00 39.17		С
ATOM	638	0	SER	A	85	49.922	40.068	12.119	1.00 39.21		0
AŢOM	639	CB	SER	Α	85	47.471	40.625	10.089	1.00 38.43		C
ATOM	640	OG	SER	Α	85	48.237	39.491	9.726	1.00 38.74		0
MOTA	641	N	ILE	Α	86	47.928	40.059	13.167	1.00 39.52		N
ATOM	642	CA	ILE	Α	86	48.348	39.116	14.192	1.00 40.46		C
ATOM	643	C	ILE	Α	8.6	48.837	37.827	13.533	1.00 41.43		С
ATOM	644	0	ILE	Α	86	49.832	37.239	13.959	1.00 41.37		0
MOTA	645	CB	ILE	A	86 -	47.179	38,792	15.155	1.00 40.12		C
MOTA	646	CG1	ILE	A	86	46.847	40.034	15.993	1.00 40.13		С
MOTA	647	CG2	ILE	A	86	47.533	37.605	16.043	1.00 39.47		С
MOTA	648	CD1	ILE	Α	86	45.631	39.878	16.891	1.00 39.39		C
MOTA	649	N	GLU		87	48.139	37.403	12.480	1.00 42.20		N
MOTA	650	CA	GLU	Α	87	48.497	36.182	11.768	1.00 42.84		C
MOTA	651	С	GLU	Α	87	49.845	36.280	11.057	1.00 42.23		C
MOTA	652	0	GLU		87	50.633	35.337	11.089	1.00 42.25		0
MOTA	653	CB .	GLU	А	87	47.405	35.809	10.755	1.00 44.28		C
ATOM	654	CG	GLU		87	46.291	36.848	10.587	1.00 46.83		C
MOTA	655	CD	GLU		87	45.454	37.041	11.847	1.00 47.87		C
ATOM	. 656		GLU		87,	44.982	36.030	12.416	1.00 48.85		0
MOTA	657	OE2	GLU		87	45.261	38.206	12.264	1.00 48.52		0
MOTA	658	И	SER		88	50.108	37.415	10.416	1.00 41.90		N
ATOM	659	CA	SER		88	51.372	37.617	9.710	1.00 41.64		C
ATOM	660	C	SER		88	52.563	37.665	10.665	1.00 40.67		C
MOTA	661	0	SER		88	53.596	37.048	10.409	1.00 40.52		0
ATOM	662	CB	SER		88	51.337	38.916	8.902	1.00 42.19		C
ATOM	663	OG	SER		88	50.359	38.853	7.882	1.00 44.49		0
MOTA	664	N	GLN		89	52.423	38.405	11.759	1.00 39.75		N
MOTA	665	CA	GLN	Α	89	53.507	38.518	12.729	1.00 39.13		С

ATOM	666	С	GLN	A	89	53.805	37.160	13.353	1.00 38.91		С
ATOM	667	0 、	GLN	A	89	54.964	36.754	13.453	1.00 38.76		0
ATOM	668	CB	${\tt GLN}$	A	89	53.151	39.534	13.821	1.00 38.26		С
MOTA	669	CG	GLN	A	89	54.226	39.689	14.888	1.00 37.37		С
ATOM	670	CD	GLN	Α	89	53.860	40.714	15.946	1.00 36.90		C
ATOM	671	OE1	GLN	Α	89	52.692	40.870	16.299	1.00 36.35		0
MOTA	672	NE2	GLN		89	54.863	41.407	16.470	1.00 36.22		N
ATOM	673	N	ALA	A	90	52.753	36.457	13.762	1.00 39.14		N
ATOM	674	CA	ALA		90	52.902	35.140	14.370	1.00 39.24		С
ATOM	675	C	ALA		90	53.587	34.185	13.395	1.00 39.46		C
ATOM	676	0	ALA		`90	54.404	33.354	13.798	1.00 39.52		Ō
ATOM	677	CB	ALA		90	51.537	34.593	14.774	1.00 39.44		C
ATOM	678	N	ALA		91	53.260	34.312	12.112	1.00 39.32		N
ATOM	679	CA	ALA		91	53.856	33.456	11.093	1.00 39.50		C
ATOM	680	C	ALA		91	55.357	33.724	10.984	1.00 39.72		C
ATOM	681	0	ALA		91	56.154	32.793	10.840	1.00 39.72		ō
ATOM	682	CB	ALA		91	53.177	33.689	9.745	1.00 39.16		С
			MET					11.045	1.00 39.10		N
MOTA	683	N			92	55.741	34.995		1.00 39.81		C
	684	CA	MET		92	57.151	35.352	10.967			
ATOM	685	C	MET		92	57.889	34.791	12.173	1.00 39.19		C
ATOM	686	0	MET		92	58.990	34.258	12.041	1.00 39.13		0
ATOM	687	CB	MET		92	57.326	36.871	10.918	1.00 40.44		C
ATOM	688	CG	MET		92	56.931	37.495	9.598	1.00 41.57		C
MOTA	689	SD	MET		92	57.352	39.245	9.523	1.00 42.86		S
MOTA	690	CE	MET		92	59.055	39.148	9.746	1.00 43.00		C
ATOM	691	N	VAL		93	57.277	34.917	13.348	1.00 38.70	•	N
MOTA	692	CA	VAL		93	57.871	34.413	14.581	1.00 38.24		C
MOTA	693	C	VÁL		93	58.066	32.909	14.452	1.00 38.82		C
MOTA	694	0	VAL	A	93	59.139	32.381	14.744	1.00 38.41	• .	0
ATOM	695	CB	LAV	А	93	56.962	34.708	15.800	1.00 37.90		С
MOTA	696	CG1	VAL	Α	93	57.400	33.883	17.003	1.00 37.53		C
MOTA	697	CG2	VAL	Α	93	57.011	36.185	16.133	1.00 37.21		С
MOTA '	698	N	HIS	Α	94	57.018	32.226	14.001	1.00 39.48		И
MOTA	699	CA	HIS	Α	94	57.061	30.778	13.828	1.00 40.12		C
ATOM	700	C	HIS	Α	94	58.181	30.377	12.866	1.00 39.88		C
MOTA	701	0	HIS	A	94	58.927	29.434	13.127	1.00 39.95		0
ATOM	702	CB	HIS	A	94	55.722	30.274	13.288	1.00 41.19		C
ATOM	703	CG	HIS	A	94	55.595	28.785	13.294	1.00 42.21		C
ATOM	704	ND1	HIS	Α	94	55.385	28.062	14.448	1.00 42.90		N
ATOM	705	CD2	HIS	A	94	55.676	27.879	12.291	1.00 42.67		С
ATOM	706	CE1	HIS	A	94	55.340	26.775	14.156	1.00 42.91		С
ATOM	707	NE2	HIS	Α	94	55.515	26.637	12.854	1.00 43.21		N
ATOM	708	N	ALA	А	95	58.294	31.104	11.759	1.00 39.52		N
MOTA	709	CA	ALA	Α	95	59.318	30.828	10.757	1.00 39.41		С
ATOM	710	С	ALA		95	60.732	30.903	11.336	1.00 39.70		С
ATOM	711	0	ALA		95	61.600	30.104	10.979	1.00 39.80		0
ATOM	712	CB	ALA		95	59.181	31.800	9.599	1.00 39.04		С
ATOM	713	N	VAL		96	60.968	31.868	12.221	1.00 39.80		И
ATOM	714	CA	VAL		96	62.280	32.022	12.834	1.00 39.46		C
ATOM	715	C	VAL		96	62.540	30.876	13.807	1.00 40.06		C
ATOM	716	Ö	VAL		96	63.640	30.322	13.851	1.00 40.00		ō
ATOM	717	СВ	VAL		96	62.392	33.367	13.593	1.00 39.16	•	C
ATOM	718		VAL		96	63.723	33.449	14.326	1.00 38.41		C
ATOM	719		VAL		96	62.264	34.522	12.617	1.00 38.80		C
ATOM	720	N	LYS		97	61.518	30.516	14.574	1.00 40.40		N
ATOM	721	CA	LYS		97	61.641	29.442	15.550	1.00 41.60		C
ATOM	722	C	LYS		97	61.861	28.063	14.927	1.00 41.00		C
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ATOM	723	0	LYS	А	97		62.472	27.193	15.548	1.00	42.73		0
ATOM	724	СВ	LYS	А	97		60.398	29.405	16.448	1.00	40.87		С
ATOM	725	CG	LYS	Α	97		60.165	30.681	17.242	1.00	39.77		.C
ATOM ·	726	CD	LYS	Α	97		61.374	31.020	18.112	1.00	38.88		С
ATOM	727	CE	LYS	A	97		61.645	29.938	19.146	1.00	38.08		. C
MOTA	728	NZ	LYS	A	97		62.859	30.238	19.957	1.00	37.01		N
ATOM	729	N	ASN	Α	98		61.373	27.867	13.705	1.00	44.37		N
ATOM	730	CA	ASN	A	98		61.509	26.579	13.024	1.00	46.53		С
ATOM	731	C	ASN	Α	98		62.485	26.602	11.854	1.00	47.31		C
ATOM	732	0	ASN	Α	98		62.519	25.664	11.056	1.00	47.58		0
ATOM	733	CB	ASN	A	98		60.146	26.112	12.506	1.00	47.72		C
ATOM	734	CG	ASN	Α	98		59.160	25.828	13.621	1.00	49.35		C
ATOM	735		ASN		98		57.953	25.977	13.439	1.00	50.61		0
ATOM	736	ND2	ASN	Α	98		59.664	25.403	14.778	1.00	49.87		N
ATOM	737	N	PHE		99		63.284	27.659	11.751	1.00			N
ATOM	738	`CA	PHE		99		64.227	27.782	10.644	1.00			C
ATOM	739	C	PHE		99		65.234	26.636	10.519	1.00			С
MOTA	740	0	PHE		99		65.528	26.189	9.412	1.00			0
ATOM	741	CB	PHE		99		64.988	29.107	10.741	1.00			С
ATOM	742	CG	PHE		99		65.802	29.425	9.518	1.00			С
ATOM	743		PHE		99		65.179	29.755	8.319	1.00		•	С
ATOM	744		PHE		99		67.192	29.383	9.559	1.00			C
ATOM	745		PHE		99		65.928	30.038	7.177	1.00			C
ATOM	746	CE2	PHE		99		67.950	29.663	8.425	1.00			.C
ATOM	747	CZ	PHE		99		67.317	29.992	7.231	1.00		•	C
ATOM	748	N	LYS				65.752	26.160	11.648	1.00		-	N
ATOM	749	CA	LYS				66.751	25.092	11.644	1.00			C
ATOM	750	C			100		66.180	23.677	11.537	1.00			C
ATOM	751	0			100		66.768	22.722	12.045	1.00			0
ATOM	752	CB	LYS				67.625	25.215	12.896	1.00			. C
ATOM	753	CG	LYS				68.234	26.604	13.048	1.00			C
ATOM	754 755	CD			100		68.860	26.837	14.417	1.00			. C
ATOM ATOM	756	CE NZ	LYS		100		70.214 70.846	26.175 26.548	14.552 15.844	1.00			N
ATOM	75 <b>7</b>	N N			101		65.041	23.543	10.864	1.00			N
ATOM	758	CA	ALA				64.402	22.241	10.691	1.00			C
ATOM	759	C	ALA				64.609	21.717	9.270	1.00			C
ATOM	760	0	ALA				64.007	22.218	8.317	1.00			0
ATOM	761	CB	ALA				62.908	22.347	10.997	1.00			C
ATOM	762	N	HIS				79.084	30.118	16.803	1.00			N
ATOM	763	CA	HIS				79.441	29.875	18.198	1.00		•	C
ATOM	764	C	HIS				78.777	30.884	19.132	1.00			C
ATOM	765	0			222		78.609	30.624	20.326	1.00			ō
ATOM	766	СВ	HIS			•	80.964	29.929	18.373	1.00			Ċ
ATOM	767	CG	HIS				81.692	28.829	17.662	1.00			Ċ
ATOM	768		HIS				81.472	27.495	17.935	1.00			N
MOTA	769		HIS				82.619	28.863	16.675	1.00			C
ATOM	770		HIS				82.231	26.755	17.145	1.00			C
ATOM	771		HIS				82.937	27.560	16.370	1.00			N
ATOM	772	N	ASN				78.399	32.036	18.588	1.00			N
ATOM	773	CA	ASN				77.749	33.058	19.391	1.00			С
ATOM	774	C	ASN				76.279	33.236	19.049	1.00			С
ATOM	775	0	ASN				75.713	34.298	19.289	1.00			0
ATOM	776	CB	ASN	A	223		78.473	34.399	19.249	1.00			С
ATOM	777	CG	ASN				79.779	34.438	20.020	1.00			C
ATOM	778	OD1	ASN	A	223		80.743	33.748	19.676	1.00	54.29		0
ATOM	779	ND2	ASN	A	223		79.815	35.244	21.078	1.00	54.20		N

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MOTA	780	N	GLU			75.657	32.201	18.490		47.90				N
ATOM	781	CA	GLU	Α	224	74.243	32.288	18.148		46.08				C
ATOM	782	C	GLU			73.406	32.282	19.418	1.00	43.99				С
MOTA	783	0	GLU	A	224	73.720	31.581	20.379	1.00	42.95				0
ATOM	784	CB -	GLU	Α	224	73.816	31.127	17.239	1.00	46.94				С
ATOM	785	CG	GLU	Α	224 .	74.134	29.736	17.778	1.00	48.84				C
ATOM	786	CD	GLU			73.590	28.616	16.896		49.60				С
ATOM	787	OE1	GLU			73.641	28.749	15.651		50.06				0
ATOM	788	OE2				73.126	27.594	17.452		49.95				ō
ATOM	789	N	LEU			72.350	33.086	19.418		42.15				N
	790	CA	LEU			71.453	33.175	20.558		40.63				C
ATOM														
MOTA	791	C	LEU			70.303	32.200	20.332		39.80				C
ATOM	792	0 .	LEU			69.475	32.407	19.445		39.10				0
ATOM	793	CB	LEU			70.915	34.600	20.692		39.95				С
ATOM	794	CG	LEU			70.043	34.870	21.920		39.53				С
ATOM	795	CD1	LEU	Α	225	70.866	34.649	23.180	1.00	39.09				С
ATOM	796	CD2	LEU	А	225	69.509	36.292	21.871	1.00	38.92				C
ATOM	797	N	VAL	Α	226	70.255	31.143	21.138	1.00	39.41				N
ATOM	798	CA	VAL	A	226	69.216	30.121	21.005	1.00	39.48				C
ATOM	799	C	VAL	Α	226	68.609	29.668	22.334	1.00	39.55				C
ATOM	800	0	VAL			69.121	29.985	23.409	1.00	39.03				0
ATOM	801	CB			226	69.772	28.859	20.301		39.18				C
ATOM	802	CG1				70.195	29.185	18.873		38.53				C
ATOM	803		VAL			70.951	28.313	21.092		39.07				C
ATOM	804	N			227	67.506	28.926	22.245		40.09				N
		CA				66.848				40.34				C
ATOM	805		ASP				28.399	23.431						
ATOM	806	C			227	67.377	26.996	23.720		41.22				C
ATOM	807	0	ASP			68.309	26.530	23.058		40.82				0
ATOM	808	CB			227	65.324	28.359	23.253		40.17				C
MOTA	809	CG			227	64.883	27.591	22.013		39.66				С
ATOM	810	OD1	ASP	Α	227	65.540	26.598	21.635		39.52				0
MOTA	811	OD2	ASP			63.851	27.975	21.424	1.00	39.07		•		0
MOTA	812	N	SER	Α	228	66.778	26.328	24.705	1.00	42.36				N
ATOM	813	CA	SER	А	228	67.190	24.979	25.098	1.00	43.39				С
ATOM	814	С	SER	A	228	67.033	23.945	23.981	1.00	44.03				C
ATOM .	815	0	SER	Α	228	67.660	22.884	24.022	1.00	44.51				0
ATOM	816	CB	SER	Α	228	66.398	24.526	26.328	1.00	43.24				C
ATOM	817	OG			228	65.008	24.504	26.053		43.57				0
ATOM	818	N			229	66.199	24.255	22.993		44.53				N
ATOM	819	CA			229	65.970	23.361	21.861		45.10				C
ATOM	820	C			229	66.852	23.748	20.676		44.98	٠.			C
ATOM	821	0			229	66.675	23.241	19.568		44.97	٠.		•	0
ATOM	822	CB			229		23.407			45.98				C
						64.497	22.870	21.431						C
ATOM	823	CG			229	63.517		22.464		47.38				C
ATOM	824	CD			229	62.069	22.994	22.014		48.68				
ATOM	825		GLN			61.684	22.476	20.962		49.59				0
ATOM	826		GLN			61.259	23.683	22.810		49.07				N
ATOM	827 -	N			230	67.793	24.657	20.919		44.98				N
ATOM	828	CA			230	68.717	25.136	19.893		44.38				C
ATOM	829	C	LYS	A	230	68.072	25.967	18.788		43.28				C,
MOTA	830	O٠			230	68.639	26.116	17.708		43.52		٠		0
MOTA	831	CB	LYS	Α	230	69.486	23.961	19.274	1.00	45.73				С
ATOM	832	CG	LYS	A	230	70.609	23.431	20.158	1.00	47.31			,	С
ATOM	833	CD			230	71.619	24.538	20.461		49.00				С
ATOM	834	CE			230	72.772	24.046	21.334		50.10				С
ATOM	835	NZ			230	73.732	25.151	21.659		50.80				N
ATOM	836	N			231	66.891	26.512	19.054		42.16				N
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ATOM	837	CA	ARG	Α	231	66.206	27.344	18.068	1.00	41.22	С
MOTA	838	С	ARG			66.596	28.797	18.324		40.06	С
ATOM	839	0	ARG			66.782	29.199	19.474		39.86	Ō
ATOM	840	СВ	ARG			64.687	27.189	18.194		42.00	Ċ
ATOM	841	CG	ARG			64.195	25.742	18.119		43.23	C
			ARG								C
MOTA	842	CD				62.693	25.651	18.341		44.06	
ATOM	843	NE	ARG			62.304	26.202	19.636		45.39	N
ATOM	844	CZ	ARG			61.047	26.309	20.058		46.06	C
MOTA	845		ARG			60.047	25.900	19.287		46.08	N
MOTA	846	NH2			231	60.787	26.833	21.251	1.00	46.43	N
MOTA	847	N	TYR	A	232	66.730	29.578	17.256	1.00	38.48	N
MOTA	848	CA	TYR	Α	232	67.093	30.985	17.390	1.00	37.00	С
MOTA	849	C	TYR	Α	232	66.068	31.733	18.236	1.00	35.83	С
MOTA	850	0	TYR	Α	232	64.867	31.475	18.154	1.00	35.57	0
ATOM	851	CB	TYR			67.183	31.656	16.015	1.00	37.19	С
MOTA	852	CG			232	68.311	31.153	15.143		37.51	С
MOTA	853	CD1				69.633	31.195	15.585		37.61	C
MOTA	854	CD2	TYR			68.058	30.636	13.872		37.62	C
MOTA	855	CE1	TYR			70.679	30.730	14.782		37.95	C
MOTA	856	CE2	TYR			69.097	30.171	13.060		37.82	C
											C
MOTA	857	CZ			232	70.400	30.219	13.521		38.06	
	858	OH	TYR			71.422	29.752	12.729		38.65	0
MOTA	859	N	LEU			66.547	32.654	19.061		34.40	N
ATOM	860	CA	LEU			65.653	33.447	19.887		33.28	C
MOTA	861	С	LEU			65.058	34.541	19.015		32.48	С
MOTA	862	0	LEU			65.681	34.992	18.053	1.00	32.36	0
MOTA	863	CB	LEU			66.418	34.080	21.057	1.00	33.73	С
MOTA	864	CG	LEU			66.128	33.504	22.449	1.00	34.07	С
MOTA	865	CD1	LEU	Α	233	66.374	32.010	22.441	1.00	33.66	С
MOTA	866	CD2	LEU	Α	233	66.994	34.190	23.496	1.00	34.12	С
MOTA	867	N	VAL	Α	234	63.842	34.958	19.335	1.00	31.40	N
MOTA	868	CA	VAL	Α	234	63.210	36.020	18.574	1.00	30.69	С
MOTA	869	С	VAL			62.213	36.752	19.447	1.00	30.26	С
ATOM	870	0	VAL			61.584	36.156	20.319		30.17	0
ATOM	871	CB	VAL			62.488	35.479	17.321		30.52	C
ATOM	872		VAL			61.272	34.654	17.719		30.18	Ċ
MOTA	873		VAL			62.083	36.636	16.434		30.21	C
ATOM	874	N	GLY			62.087	38.052	19.218		30.07	N
ATOM	875	CA	GLY			61.158	38.851	19.987		29.43	C
ATOM	876	C					39.341			29.43	C
			GLY GLY			60.039		19.095 17.874			
ATOM	877	0				60.105	39.201			29.17	0
MOTA	878	N	ALA			59.011	39.922	19.699		28.71	N
ATOM	879	CA	ALA			57.888	40.420	18.929		28.71	C
MOTA	880	C	ALA			57.267	41.637	19.600		28.78	C
MOTA	881	0	ALA			57.035	41.643	20.809		28.79	0
MOTA	882	CB	ALA			56.846	39.320	18.768		28.81	С
MOTA	883	N	GLY			57.007	42.670	18.809		28.64	N
ATOM	884	CA	GLY			56.405	43.866	19.355	1.00	28.99	C
MOTA	885	С	GLY			54.902	43.715	19.462	1.00	29.51	, C
MOTA	886	0	$\operatorname{GLY}$	A	237	54.284	43.014	18.657	1.00	29.85	0
MOTA	887	N	ILE	A	238	54.311	44.352	20.467	1.00	29.44	N
ATOM	888	CA	ILE			52.866	44.301	20.649		29.75	С
MOTA	889	C.			238	52.370	45.707	20.959		30.10	C
ATOM	890	0	ILE			53.150	46.580	21.332		29.88	0
ATOM	891	CB	ILE			52.449	43.359	21.814		29.59	Ċ
ATOM	892	CG1				52.950	43.912	23.151		29.43	C
ATOM	893		ILE			53.001	41.964	21.578		29.87	C
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MOTA	894	CD1	ILE	Α	238	52.438	43.149	24.376	1.00	28.69		С
ATOM	895	N	ASN	А	239	51.072	45.925	20.789	1.00	30.32		N
MOTA	896	CA	ASN	Α	239	50.488	47.224	21.067	1.00	30.41		C
MOTA	897	C	ASN	А	239	49.515	47.095	22.233	1.00	30.69		С
ATOM	898	0	ASN	Α	239	49.107	45.992	22.599	1.00	30.13		0
ATOM ·	899	CB	ASN	Α	239 .	49.774	47.760	19.822	1.00	30.86		С
ATOM	900	CG	ASN	Α	239	48.606	46.892	19.397	1.00	30.89		С
MOTA	901	OD1	ASN	Α	239	47.610	46.785	20.108	1.00	30.90		0
ATOM	902	ND2	ASN	Α	239	48.724	46.269	18.231	1.00	31.26		N
ATOM	903	N	THR			49.144	48.226	22.816	1.00	31.46	4	N
ATOM	904	CA	THR		· ·	48.236	48.229	23.953	1.00	32.48		С
ATOM	905	С	THR			46.760	48.143	23.557	1.00	33.71		. C
ATOM	906	0	THR			45.885	48.393	24.383	1.00	33.65		0
ATOM	907	CB	THR			48.448	49.491	24.792	1.00	32.03		С
ATOM	908	OG1				48.264		23.957		31.61		0
ATOM	909		THR			49.862		25.366		31.27		C
ATOM	910	N	ARG			46.484	47.782	22.305		34.92		N
ATOM	911.	CA	ARG			45.100	47.680	21.837		36.67		C
ATOM	912	C	ARG			44.578	46.259	21.614		36.73		Ċ
ATOM	913	0	ARG			43.619	45.848	22.262		36.77		ō
ATOM	914	CB	ARG			44.909	48.494	20.552		37.87		C
ATOM	915	CG	ARG			44.891	50.010	20.755		40.48		C
ATOM	916	CD	ARG			44.875	50.729	19.409		42.72		C
ATOM	917	NE	ARG			44.876	52.188	19.522		44.49		N
ATOM	918	CZ	ARG			43.818	52.916	19.866		45.58		C
ATOM	919		ARG			42.661	52.325	20.140		46.47		N
ATOM	920		ARG			43.909	54.239	19.912		45.69		N
ATOM	921	N	ASP			45.202	45.505	20.713		36.96		N
ATOM	922	CA	ASP			44.732	44.148	20.713		37.70		C
ATOM	923	C	ASP			45.537	43.008	21.051	-	37.72		C
ATOM	924	0	ASP			45.525	41.888	20.540		38.14		0
MOTA	925	CB	ASP			44.663	43.927	18.904		37.89		. C
MOTA	926	CG	ASP			46.025	44.024	18.225		38.50		C
MOTA	927		ASP				43.712			38.41		
MOTA	928		ASP			47055		18.866				0
MOTA	929	N N	PHE			46.066	44.394	17.029		38.58 37.60		- O
ATOM		CA	PHE			46.210	43.287	22.163 22.838		•		N.
	930 931	CA	PHE			47.043	42.293	23.339		37.44		C
MOTA			PHE			46.355				37.84		
MOTA MOTA	932 933	O CB	PHE			46.992	39.970 42.957	23.425		37.47	•	0
	934	CG				47.796 46.903		23.996		36.54		C
ATOM			PHE				43.587	25.022		35.45		C
MOTA	935		PHE			46.382	42.833	26.066		35.41		C
ATOM	936					46.594	44.940	24.955		35.12		C
ATOM	937		PHE			45.566	43.416	27.033		34.98		C
ATOM	938		PHE			45.780	45.534	25.916		35.22		C
MOTA	939	CZ	PHE			45.265	44.769	26.959		35.05		C
ATOM	940	N	ARG			45.072	41.114	23.675		38.36		И
ATOM	941	CA	ARG			44.337	39.949	24.163		38.96		C
ATOM		C	ARG			44.291	38.857	23.099		39.31		C
ATOM	943	0	ARG			44.140	37.676	23.413		39.37		O
ATOM	944	CB	ARG			42.913	40.340	24.579		38.87		C
MOTA	945	CG	ARG			42.863	41.345	25.722		38.92		C
ATOM	946	CD	ARG			41.440	41.607	26.189		38.85		C
ATOM	947	NE	ARG			41.389	42.595	27.267		39.27		N
ATOM	948	CZ	ARG			41.572	43.902	27.095		39.54		C.
ATOM	949		ARG			41.816	44.388	25.885		39.23		N
ATOM	950	NH2	ARG	А	∠44	41.510	44.725	28.135	1.00	39.60		N

MOT! K	951	NT	CTI	7	245		44.422	39.257	21.839	1 00	39.62	N
ATOM		N			245							N
MOTA	952	CA			245		44.413	38.300	20.742		39.94	С
MOTA	953	C			245		45.822	38.091	20.183		39.41	С
MOTA	954	0	GLU	A	245		46.214	36.965	19.873	1.00	39.17	0
MOTA	955	CÉ	GLU	·Α	245		43.477	38.772	19.618	1.00	41.18	C
ATOM	956	CG	GLU	A	245		41.987	38.670	19.955	1.00	43.82	C
MOTA	957	CD			245		41.479	39.800	20.848	1.00	45.62	· C
ATOM	958	OE1					40.433	39.604	21.510		46.25	0
	959		GLU				42.105	40.889	20.881		46.89	0
ATOM												
ATOM	960	N			246		46.584	39.177	20.067		38.53	N
MOTA	961	CA			246		47.940	39.103	19.528	1.00	37.66	С
MOTA	962	С	ARG	Α	246		48.908	38.320	20.415	1.00	37.14	С
ATOM .	963	0	ARG	Α	246		49.651	37.469	19.931	1.00	37.14	0
ATOM	964	CB	ARG	Α	246		48.490	40.516	19.287	1.00	36.94	С
ATOM	965	CG	ARG	Α	246		49.819	40.546	18.536	1.00	36.46	С
ATOM	966	CD			246		50.278	41.970	18.276		35.96	. С
ATOM	967	NE			246		49.341	42.724	17.441		35.46	N
ATOM	968	CZ			246		49.311	42.687	16.111		35.16	Č
MOTA	969		ARG					41.932	15.441		34.77	N
MOTA	970	NH2	ARG				48.421	43.417	-15.448		35.59	N
MOTA	971	N			247		48.896	38.599	21.714	1.00	36.70	N
MOTA	972	CA	VAL	Α	247		49.802	37.919	22.630	1.00	36.48	C
ATOM	973	C	VAL	Α	247		49.701	36.389	22.572	1.00	36.82	C
ATOM	974	0			247		50.702	35.710	22.328	1.00	36.60	0
ATOM	975	СВ			247		49.589	38.404	24.087		35.99	C
ATOM	976		VAL				50.425	37.578	25.042		35.65	c
ATOM	977		VAL				49.969	39.877	24.202		35.85	C
ATOM	978	N			248		48.497	35.824	22.800		36.88	N
MOTA	979	CA			248		48.355	34.363	22.756		36.60	C
MOTA	980	C	PRO	A	248		48.891	33.775	21.453		36.20	С
MOTA	981	0	PRO	A	248		49.538	32.729	.21.450	1.00	36.15	0
MOTA	982	CB	PRO	Α	248		46.850	34.163	22.920	1.00	36.98	C
ATOM	983	CG	PRO	Α	248		46.469	35.306	23.823	1.00	36.81	C
ATOM	984	CD	PRO	Α	248		47.223	36.459	23.192	1.00	36.48	С
ATOM	985	N			249		48.626	34.465	20.349	1.00	36.16	N
ATOM	986	CA			249			34.025	19.042		36.32	c
ATOM	987	C			249		50.613	34.043	19.000		36.64	c
	988	0									36.51	0
ATOM					249		51.242	33.137	18.444			
ATOM	989		ALA				48.517	34.931	17.959		36.44	C
ATOM	990	N			250		51.206	35.076	19.596		36.66	N
ATOM	991	CA			250		52.660	35.202	19.629		36.66	C
ATOM	992 ,	C	LEU	Α	250		53.284	34.148	20.540	1.00	36.79	С
ATOM	993	0	LEU	А	250		54.328	33.586	20.222	1.00	36.30	0
MOTA	994 ~	CB	LEU	Α	250		53.062	36.610	20.090	1.00	36.33	C
MOTA	995	CG	LEU	Α	250		53.366	37.679	19.026	1.00	36.54	, C
ATOM	996		LEU				52.849	37.266	17.658		36.13	Ċ
MOTA	997		LEU				52.757	39.002	19.461		35.88	C
ATOM	998	N			251		52.644	33.878	21.671		37.78	N
ATOM	999	CA										
					251	•	53.166	32.875	22.593		39.09	C
ATOM	1000	C			251		53.103	31.507	21.928		39.91	C
ATOM	1001	0			251		54.069	30.745	21.961		40.18	0
ATOM	1002	CB					52.358	32.829	23.907		38.94	· C
MOTA	1003	CG1	VAL	A	251		52.815	31.651	24.761	1.00	39.25	C
MOTA	1004	CG2	VAL	Α	251		52.545	34.126	24.674	1.00	39.03	С
MOTA	1005	N	GLU	Α	252		51.963	31.200	21.317	1.00	40.90	N
MOTA	1006	CA			252		51.794	29.918	20.642		41.65	C
ATOM	1007	С			252		52.801	29.762	19.504		40.64	C
		-		-							· - ·	-

ATOM	1008	0	GLU	Α	252	53.293	28.666	19.251	1.00	40.83			0
MOTA	1009	CB	GLU			50.370	29.784	20.095		43.45			С
ATOM	1010	CG	GLU			49.477	28.839	20.889		46.51			C
ATOM	1011	CD	GLU			49.239	29.298	22.318		48.31			C
ATOM	1012		GLU			48.600	30.359	22.512		49.25			0
			GLU				28.589	23.249					0
ATOM	1013	OE2				49.691				49.10			
MOTA	1014	N	ALA			53.103	30.864	18.822		39.42			N
MOTA	1015	CA	ALA			54.051	30.844	17.714		38.09			С
MOTA	1016	C	ALA			55.488	30.617	18.189		37.51			С
MOTA	1017	0	ALA	A	253	56.377	30.344	17.380	1.00	37.32		•	0
MOTA	1018	CB	ALA	А	253	53.961	32.137	16.931	1.00	37.90			C
ATOM	1019	N	GLY	Α	254	55.715	30.740	19.495	1.00	36.62			N
MOTA	1020	CA	GLY	A	254	57.048	30.521	20.033	1.00	35.88			С
MOTA	1021	C	GLY			57.879	31.754	20.366	1.00	35.36			C
ATOM	1022	0			254	59.072	31.632	20.651		34.95			0
ATOM	1023	N	ALA			57.270	32.938	20.330		34.50			N
ATOM	1023	CA				57.270	34.166	20.530		33.48			C
			ALA										
MOTA	1025	C	ALA			58.659	34.025	22.019		32.88			С
MOTA	1026	0	ALA			58.016	33.663	23.000		32.47			0
MOTA	1027	CB	ALA			57.039	35.352	20.644.			٠,		C
MOTA	1028	N	ASP	Α	256	59.954	34.309	22.079	1.00	32.31	•		N
MOTA	1029	CA	ASP	A	256	60.703	34.185	23.323	1.00	31.81			C
ATOM	1030	C	ASP	A	256	60.518	35.367	24.266	1.00	31.12			C
MOTA	1031	0	ASP	Α	256	60.649	35.232	25.481	1.00	30.65			0
MOTA	1032	CB	ASP	A	256	62.181	33.994	22.999	1.00	31.98			С
ATOM	1033	CG	ASP			62.425	32.745	22.182		32.65			C
MOTA	1034		ASP			62.295	31.643	22.749		33.20			0
MOTA	1035		ASP			62.725	32.860	20.975		32.82			0
ATOM	1036	N	VAL			60.211	36.526	23.700		30.48			N
MOTA	1037	CA	VAL			60.007	37.722	24.500		29.85			C
MOTA	1038	C	VAL		and the second s	59.153	38.696	23.708		29.52			C
ATOM	1039	0	VAL			59.158	38.683	22.477		29.18			0
MOTA	1040	CB	VAL			61.359	38.398	24.867		29.74			С
MOTA	1041	CG1	VAL	A	257	62.118	38.768	23.603	1.00	29.96			С
ATOM	1042	CG2	VAL	Α	257	61.116	39.636	25.721	1.00	29.25			С
MOTA	1043	N	LEU	Α	258	58.410	39.530	24.422	1.00	28.83			N
ATOM	1044	CA	LEU	Α	258	57.556	40.513	23.785	1.00	28.70			С
ATOM	1045	C	LEU	Α	258	57.993	41.899	24.238	1.00	28.49			C
MOTA	1046	0	LEU			58.752	42.041	25.198		28.65			0
MOTA	1047	СВ	LEU			56.094	40.289	24.189		28.62			C
	1048	CG	LEU				38.871	24.065		29.10			Ċ
ATOM	1049		LEU			54.122	38.855	24.605		29.34			C
										29.01			
MOTA	1050		LEU		,	55.573	38.407	22.610					C
MOTA	1051	N			259	57.527	42.920	23.535		27.96			N
MOTA	1052	CA			259	57.840	44.286	23.914		27.94		•	C
MOTA	1053	C			259	56.759	45.216	23.403		27.70			C
MOTA	1054	0			259	56.475	45.257	22.209		27.35			0
MOTA	1055	CB	CYS	Α	259	59.198	44.730	23.358		27.38			С
ATOM	1056	SG	CYS	Α	259	59.725	46.331	24.021	1.00	26.82			S
MOTA	1057	N	ILE	Α	260	56.143	45.950	24.320	1.00	28.21			N
MOTA	1058	CA	ILE	А	260	55.108	46.898	23.943	1.00	28.49			C
ATOM	1059	С			260	55.815	48.001	23.168		29.26			С
MOTA	1060	0			260	56.769	48.615	23.657		28.86	•		Ō
ATOM	1061	СВ			260	54.421	47.483	25.182		28.21			C
ATOM	1062		ILE			53.792	46.346	25.102		27.85			C
MOTA	1062		ILE			53.732	48.510	24.761		27.76			C
													C
MOTA	1064	דער	ILE	H	∠0U	53.275	46.763	27.351	1.00	27.51			C

MOTA	1065	N	ASP	A	261	55.344	48.233	21.951	1.00	29.87		N
MOTA	1066	CA	ASP	Α	261	55.920	49.224	21.062	1.00	30.69		C
MOTA	1067	C	ASP	A	261	55.160	50.552	21.108	1.00	31.35		C
MOTA	1068	0	ASP	A	261	54.046	50.659	20.597	1.00	31.90		0
MOTA	1069	CB	ASP	Α	261 ·	55.934	48.632	19.651	1.00	31.21		С
ATOM	1070	CG	ASP			56.417	49.603	18.599		31.62		С
ATOM	1071		ASP			57.220	50.508	18.913		31.79		ō
ATOM	1072		ASP			55.997	49.438	17.437		32.40		0
ATOM	1072	N	SER			55.767	51.562	21.727		31.57		N.
							52.876					
MOTA	1074	CA	SER			55.136		21.843		32.25		C
ATOM	1075	C ·	SER			56.162	53.984	22.056		32.15		C
ATOM	1076	0	SER			57.250	53.730	22.574		32.40		0
MOTA	1077	СВ	SER			54.146	52.871	23.012		32.42		С
ATOM	1078	OG	SER			53.637	54.171	23.261		33.43		0
MOTA	1079	N	SER			55.818	55.212	21.665	1.00	31.88		И
MOTA	1080	CA	SER	Α	263	56.734	56.331	21.847	1.00	31.98		C
MOTA	1081	C	SER	A	263	56.658	56.839	23.280	1.00	31.45		С
MOTA	1082	0	SER	Α	263	57.683	57.118	23.898	1.00	32.24		0
ATOM	1083	CB	SER	Α	263	56.433	57.465	20.859	1.00	32.64		C
MOTA	1084	OG	SER	Α	263	55.121	57.971	20.999	1.00	35.89		0
ATOM	1085	N	ASP			55.447	56.941	23.814	1.00	30.33		N
MOTA	1086	CA	ASP			55.253	57.394	25.189		29.38		C
ATOM	1087	C	ASP			54.694	56.241	26.026		28.76		C
	1088	Ō			264	53.481	56.036	26.093		28.66		0
MOTA	1089	CB	ASP			54.298	58.597	25.215		29.24		C
ATOM	1090	CG	ASP				59.037	26.632		29.06		C
						53.927						
ATOM	1091		ASP			54.618	58.666	27.606		28.24		0
ATOM	1092		ASP			52.935	59.780	26.763		28.61		0
ATOM	1093	N	GLY			55.594	55.497	26.664		27.72		N.
MOTA	1094	CA	GLY			55.194	54.358	27.474		26.80		C
ATOM	1095	C	GLY			54.724	54.700	28.874	1.00	26.32		С
ATOM	1096	0	GLY	А	265	54.304	53.815	29.622	1.00	25.26		0
MOTA	1097	N	PHE	Α	266	54.800	55.978	29.238	1.00	26.32		И
MOTA	1098	CA	PHE	Α	266	54.358	56.418	30.555	1.00	26.48		C
MOTA	1099	C	PHE	Α	266	52.841	56.551	30.402	1.00	27.26		C
ATOM	1100	0	PHE	Α	266	52.277	57.642	30.427	1.00	26.89		0
ATOM	1101	CB-	PHE	Α	266	55.000	57.764	30.903	1.00	26.26		C
MOTA	1102	CG	PHE	Α	266	55.074	58.045	32.388	1.00	26.33		C
ATOM	1103		PHE			54.336	57.289	33.301		25.12		C
MOTA	1104		PHE			55.866	59.089	32.867		25.66		Ċ
ATOM	1105		PHE			54.385	57.569	34.664		25.49.		C
ATOM	1106		PHE		P	55.922	59.378	34.228		24.95		C
MOTA	1107	CZ			266	55.179	58.617	35.131		25.18		C
MOTA	1107				267	52.195						
		N					55.403	30.239		28.41		N
ATOM	1109	CA			267	50.764	55.334	30.010		29.17		C
MOTA	1110	C			267	50.084	54.224	30.791		29.72		С
ATOM	1111	0			267	50.659	53.155	31.012		29.22		0
MOTA	1112	CB			267	50.515	55.112	28.521		29.55		C
MOTA	1113	OG			267·	49.162	54.792	28.269		31.97		0
ATOM	1114	N			268	48.844	54.482	31.188		30.02		N
MOTA	1115	CA			268	48.072	53.506	31.927		31.13		С
ATOM	1116	C	GLU	A	268	47.767	52.325	31.005	1.00	31.03		С
ATOM	1117	0	GLU	A	268	47.618	51.195	31.462	1.00	30.56		0
MOTA	1118	CB	GLU	A	268	46.775	54.139	32.437	1.00	32.14		С
ATOM	1119	CG	GLU	А	268	45.961	53.213	33.322	1.00	34.23		С
MOTA	1120	CD			268	44.724	53.872	33.902		35.72		С
ATOM	1121	OE1	GLU			43.933	53.148	34.551		36.93		0
				-	•		·					-

MOTA	1122	OE2	GLU	Α	268	44.542	55.099	33.717	1.00	35.59		0
ATOM	1123	N	TRP	A	269	47.688	52.592	29.703	1.00	31.57		N
MOTA	1124	CA	TRP	A	269	47.414	51.539	28.730	1.00	32.18		С
ATOM	1125	C	TRP	A	269	48.488	50.453	28.800	1.00	32.07		С
MOTA	1126	0			269	48.194	49.266	28.661	1.00	32.37		0
MOTA	1127	CB	TRP	A	269	47.347	52.109	27.309	1.00	32.84		C
MOTA	1128	CG	TRP	Α	269	46.211	53.064	27.085	1.00	34.12		С
MOTA	1129	CD1	TRP	A	269	46.306	54.401	26.827	1.00	34.63		C
MOTA	1130	CD2	TRP	Α	269	44.807	52.761	27.114	1.00	34.88		C
MOTA	1131	NE1	TRP	A	269	45.051	54.950	26.694	1.00	35.25		N
MOTA	1132	CE2	TRP	A	269	44.114	53.966	26.866	1.00	34.78		C
ATOM	1133	CE3			269	44.068	51.587	27.325	1.00	35.27		C
MOTA	1134	CZ2	TRP	A	269	42.717	54.035	. 26.823 -	1.00	35.56		C
MOTA	1135	CZ3	TRP	Α	269	42.675	51.655	27.284	1.00	35.55		С
MOTA	1136	CH2	TRP	Α	269	42.017	52.872	27.035	1.00	35.57		C
MOTA	1137	N			270	49.736	50.855	29.013	1.00	31.69		N
ATOM	1138	CA	GLN	А	270	50.808	49.875	29.114		31.74		C
ATOM	1139	C -	GLN	А	270	50.720	49.115	30.430		31.80		С
MOTA	1140	0			270	51.002	47.916	30.480		32.05		0
MOTA	.1141	CB			270	52.179	50.544	28.965		30.95		С
MOTA	1142	CG			270	52.461	50.929	27.526	1.00	30.42		C
MOTA	1143	CD			270	53.936	50.960	27.191		29.71		С
MOTA	1144	OE1			270	54.755	50.317	27.851		28.19		0
ATOM	1145	NE2			270 .	54.278	51.691	26.141		28.75		N
MOTA	1146	N			271	50.325	49.803	31.495		31.92		N
MOTA	1147	CA			271	50.192	49.138	32.781		32.22		C
MOTA	1148	C			271	49.114	48.065	32.643		31.72		C
MOTA	1149	0			271	49.265	46.949	33.135		31.50		0
MOTA	1150	CB			271	49.795	50.131	33.872		32.96		C
ATOM	1151	CG			271	49.476	49.448	35.190		34.60		C
ATOM	1152	CD			271	49.184	50.433	36.301		36.08	•	C
ATOM	1153	CE	LYS			48.928	49.688	37.605		37.48		C
MOTA	1154	ΝZ			271	48.792	50.615	38.769		39.24		N
MOTA	1155	N			272	48.031	48.421	31.959		31.65		N
ATOM	1156	CA			272	46.919	47.511	31.733		31.59		C
ATOM	1157	C			272	47.351	46.309	30.904		31.68		C
ATOM	1158	0			272	46.967	45.182	31.203		31.84		0
ATOM	1159	CB			272	45.751	48.232	31.025		31.59		C
MOTA	1160	CGI	ILE			45.058	49.167	32.018		30.96		C
MOTA	1161 1162	CG2			272	44.761	47.214	30.452		31.15		C
MOTA MOTA	1163	CD1			272	44.109	50.157 46.548	31.367 29.869		30.73		C
MOTA	1164	N CA			273	48.151	45.465	29.015		31.76		N C
ATOM	1165	CA			273	49.536	44.497	29.788		32.26		C
ATOM	1166	0			273	49.374	43.280	29.695		32.32		0
MOTA	1167	CB			273	49.406	46.020	27.806		32.10		C
MOTA	1168	OG1			273	48.522	46.813	27.004		32.10		0
MOTA	1169	CG2			273	49.970	44.890	26.960		32.28		C
MOTA	1170	N			274	50.487	45.030	30.548		32.22		N
MOTA	1171	CA			274	51.377	44.176	31.328		32.21		C
ATOM	1172	C			274	50.558	43.401	32.366		32.57		C
ATOM	1173	0			274	50.783	42.212	32.590		32.28		0
MOTA	1174	CB			274	52.445	44.999	32.071		31.88		C
ATOM	1175	CG1			274		45.802	31.070		31.35		C
MOTA	1176		ILE			53.332	44.068	32.899		31.40		C
MOTA	1177		ILE			54.276	46.749	31.724		31.35		C
ATOM	1178	N			275	49.610	44.089	32.994		32.79		N
	•											

ATOM	1179	CA	GLY	Α	275	48.772	43.454	33.994	1.00	33.65		С
ATOM	1180	C	GLY			47.998	42.274	33.438		33.76		C
ATOM	1181	0	GLY			47.845	41.251	34.103		34.32		Ō
ATOM	1182	N	TRP			47.505	42.412	32.214		33.77		N
												C
ATOM	1183	CA	TRP			46.752	41.341	31.580		34.23		
MOTA	1184	C	TRP			47.677	40.152	31.331		34.65		C
	.1185	0	TRP			47.293	39.001	31.536		34.89		0
MOTA	1186	CB	TRP			46.163	41.821	30.253		34.33		С
ATOM	1187	CG	TRP	A	276	45.278	40.809	29.591	1.00	34.90		С
MOTA	1188	CD1	TRP	A	276	43.932	40.639	29.784	1.00	34.76		C
MOTA	1189	CD2	TRP	Α	276	45.675	39.817	28.635	1.00	34.98		C
ATOM	1190	NE1	TRP	Α	276	43.469	39.604	29.003	1.00	34.35		N
ATOM	1191	CE2	TRP	Α	276	44.516	39.082	28.289	1.00	34.87		C
ATOM	1192	CE3	TRP	Α	276	46.898	39.476	28.038	1.00	35.16		C
MOTA	1193	CZ2	TRP			44.545	38.026	27.368	1.00	35.33		С
MOTA	1194	CZ3	TRP			46.927	38.425	27.122		35.14		С
ATOM	1195	CH2	TRP			45.755	37.713	26.797		35.58		C
MOTA	1196	N			277	48.900	40.435	30.890		34.66		N
MOTA	1197	CA			277	49.868	39.381	30.620		34.37		C
MOTA	1198	C			277	50.227	38.622	31.900		35.02		C
					277 .		37.399			34.44		0
MOTA	1199	0				50.350		31.891				
ATOM	1200	CB			277	51.146	39.961	29.972		33.65		C
ATOM	1201		ILE			50.802	40.550	28.604		33.07		C
ATOM	1202	CG2	ILE			52.206	38.877	29.823		32.69		C
MOTA	1203		ILE			51.952	41.268	27.926		32.85		C
MOTA	1204	N	ARG			50.390	39.346	33.001		36.08		N
MOTA	1205	CA	ARG			50.722	38.713	34.275		37.93	•	C
MOTA	1206	C -	ARG	Α	278	49.570	37.835	34.757	1.00	39.10		С
MOTA	1207	0	ARG	А	278	49.778	36.704	35.192	1.00	39.55		0
MOTA	1208	CB	ARG	Α	278	51.037	39.774	35.334	1.00	37.11		C
MOTA	1209	CG	ARG	A	278	52.342	40.499	35.106	1.00	36.58		С
MOTA	1210	CD	ARG	Α	278	53.533	39.574	35.306	1.00	36.31		C
MOTA	1211	NE	ARG	A	278	54.770	40.224	34.883	1.00	35.73		N
MOTA	1212	CZ	ARG	Α	278	55.478	39.861	33.819	1.00	35.12		С
MOTA	1213	NH1	ARG	Α	278	55.079	38.840	33.072	1.00	33.98		N
MOTA	1214	NH2	ARG			56.569	40.539	33.487		34.31		N
MOTA	1215	N	GLU			48.356	38.367	34.669		40.86		N
ATOM	1216	CA	GLU			47.157	37.654	35.089		42.25		C
ATOM	1217	C	GLU			46.961	36.339	34.331		42.65		C
ATOM	1218	0	GLU			46.500	35.352	34.900		42.50		0
ATOM	1219	СВ	GLU			45.931	38.556	34.894		43.71		C
ATOM	1220	CG			279	44.582	37.864	35.074		46.30	•	C
ATOM	1221	CD			279	43.398	38.825	34.946		48.03	•	C
MOTA	1222		GLU			43.314	39.555	33.928		48.89		0
ATOM	1223	OE2				42.544	38.844	35.863		48.40		0
MOTA	1224	N			280	47.324	36.319	33.055		42.53		N
ATOM	1225	CA			280'	47.144	35.116	32.255		42.83		C
MOTA	1226	C			280	48.356	34.188	32.182		42.50		С
ATOM	1227	0			280	48.201	32.975	32.047		42.55		0
MOTA	1228	CB			280	46.723	35.499	30.834		43.85		C
MOTA	1229	CG			280	46.229	34.321	30.008		45.53		C
MOTA	1230	CD	LYS	Α	280	45.821	34.743	28.602	1.00	46.52		С
MOTA	1231	CE	LYS	A	280	45.103	33.612	27.871	1.00	46.76		С
MOTA	1232	NZ	LYS	A	280	45.916	32.367	27.837	1.00	47.35		· N
MOTA	1233	N	TYR	A	281	49.557	34.749	32.287	1.00	41.56		N
MOTA	1234	CA			281	50.771	33.949	32.172		40.39		C
MOTA	1235	C			281	51.738	34.039	33.341		40.00		С

MOTA	1236	0	TYR	A	281	52.746	33.335	33.360	1.00 39	.98	0
ATOM	1237	CB	TYR	Α	281	51.530	34.355	30.910	1.00 40	.02	С
ATOM	1238	CG	TYR	A	281	50.757	34.204	29.625	1.00 39	.56	С
MOTA	1239	CD1	TYR	A	281	50.552	32.949	29.056	1.00 39	.41	C
MOTA	1240	CD2	TYR	Α	281	50.255	35.322	28.957	1.00 39	.51	С
MOTA	1241	CE1	TYR			49.873	32.809	27.853	1.00 39	.24	С
MOTA	1242	CE2	TYR			49.571	35.193	27.752	1.00 39		С
MOTA	1243	CZ	TYR			49.386	33.933	27.206	1.00 39		С
MOTA	1244	OH	TYR			48.722	33.794	26.012	1.00 39		Ó
ATOM	1245	N	GLY			51.444	34.892	34.313	1.00 39		N
ATOM	1246	CA	GLY			52.365	35.045	35.422	1.00 39		C
ATOM	1247	C .	GLY			53.673	35.588	34.863	1.00 39		C
ATOM	1248	0	GLY			53.665	36.379	33.916	1.00 39		ō
MOTA	1249	N	ASP			54.796	35.156	35.427	1.00 39		N
ATOM	1250	CA	ASP			56.105	35.611	34.968	1.00 40		C
MOTA	1251	C	ASP			56.709	34.682	33.916	1.00 39		C
MOTA	1252	Ō	ASP			57.905	34.745	33.638	1.00 40		ō
MOTA	1253	CB	ASP			57.063	35.737	36.157	1.00 41		c
ATOM	1254	CG	ASP			56.660	36.845	37.118	1.00 42		C
ATOM	1255		ASP			56.621	38.024	36.696	1.00 43		0
ATOM	1256		ASP			56.381	36.541	38.300	1.00 43		0
ATOM	1257	N	LYS			55.882	33.825	33.328	1.00 39		N
ATOM	1258	CA	LYS		,	56.354	32.887	32.314	1.00 39		C
ATOM	1259	C	LYS			56.482	33.538	30.937	1.00 37		C
ATOM	1260	0	·LYS			57.178	33.026	30.061	1.00 37		0
MOTA	1261	CB	LYS			55.416	31.678	32.234	1.00 40		C
ATOM	1262	CG	LYS		-	55.327	30.866	33.526	1.00 40		C
ATOM	1263	CD	LYS			56.686	30.300	33.930	1.00 42		C
ATOM	1264	CE	LYS			56.559	29.340	35.112	1.00 44		C
ATOM	1265	NZ	LYS			57.886	28.778	35.524	1.00 45		N
ATOM	1266	N	VAL			55.793	34.655	30.741	1.00 40		N
ATOM	1267	CA	VAL			55.863	35.383	29.482	1.00 34		C
ATOM	1268	C	VAL			56.556	36.709	29.781	1.00 34		C
ATOM	1269	0	VAL								
ATOM	1209	CB	VAL			56.094	37.486 35.630	30.619 28.899	1.00 32		O C
ATOM	1271	CG1				54.453 54.520	36.625	27.749	1.00 33		C
ATOM	1272		VAL			53.868	34.311	28.408	1.00 33		C
ATOM .	1272	N N	LYS			57.676	36.951	29.108	1.00 33		N
ATOM		CA	LYS			58.457	38.171	29.313	1.00 32	4.5	C
ATOM	1275	C	LYS			57.988	39.305	28.407	1.00 31		C
ATOM	1276	0	LYS			57.751	39.107	27.216			
ATOM	1277	CB			286	59.943	37.885	29.067	1.00 29 1.00 31		O C
ATOM	1278	CG			286	60.484	36.696		1.00 31		C
ATOM	1279	CD			286	60.260	36.865	29.857 31.357	1.00 31		C
ATOM	1280	CE	LYS			60.845	35.697	32.145	1.00 31		C
ATOM	1280	NZ	LYS					33.619			
ATOM	1282	N	VAL			60.578 57.858	35.811 40.498	28.980	1.00 31		N
ATOM	1283	CA			287	57.402			1.00 28		N C
	1284						41.649	28.218			
ATOM ATOM	1285	C 0	VAL		287	58.123	42.952 43.395	28.571 29.723	1.00 28		С О
ATOM	1285	CB	VAL			58:116			1.00 28		
			VAL			55.870	41.843	28.397	1.00 29		C
MOTA MOTA	1287 1288					55.514	41.886	29.873			C
ATOM			VAL			55.417	43.120	27.721	1,00 28		C
ATOM	1289	N CA	GLY			58.754	43.555	27.568	1.00 27		N C
ATOM	1290 1291	CA	GLY			59.441	44.817	27.771	1.00 26		C
ATOM	1291	0 .	GLY GLY			58.434	45.938	27.573	1.00 26		0
-11 014	1636	9	GUI	М	200	57.403	45.737	26.922	1.00 26		J

MOTA	1293	N	ALA	A	289	58.721	47.112	28.128	1.00 26.17	N
ATOM	1294	CA	ALA	Α	289	57.820	48.255	28.012	1.00 26.19	C
ATOM	1295	С	ALA	A	289	58.591	49.543	27.741	1.00 26.50	C
ATOM	1296	0	ALA	A	289	59.810	49.593	27.900	1.00 26.69	0
ATOM	1297	CB	ALA			56.994	48.401	29.291	1.00 26.59	C
ATOM	1298	N	GLY			57.871	50.584	27.331	1.00 26.15	
MOTA	1299	CA	GLY			58.502	51.856	27.037	1.00 25.55	
ATOM	1300	C	GLY			57.745	52.567	25.930	1.00 25.64	
ATOM	1301	0	GLY			56.726	52.059	25.470	1.00 25.93	
ATOM	1302	N	ASN			58.246	53.712	25.468	1.00 24.68	
		CA	ASN					25.961	1.00 24.00	
ATOM	1303		ASN			59.491	54.295	27.022		
ATOM	1304	C				59.309	55.373		1.00 23.88	
MOTA	1305	0	ASN			58.278	56.041	27.078	1.00 24.05	
ATOM	1306	CB	ASN			60.279	54.883	24.788	1.00 23.44	
MOTA	1307	CG	ASN			60.771	53.819	23.840	1.00 24.01	
MOTA	1308		ASN			60.266	52.695	23.849	1.00 24.09	
MOTA	1309		ASN			61.756	54.162	23.012	1.00 22.58	
MOTA	1310	N				60.323	55.522	27.867	1.00 23.43	
ATOM .	1311	CA	ILE	A	292	60.329	56.541	28.906	1.00 23.67	
MOTA	1312	С	ILE	Α	292	61.706	57.220	28.861	1.00 23.76	, C
MOTA	1313	0	ILE	Α	292	62.642	56.688	28.247	1.00 23.31	
MOTA	1314	CB	ILE	А	292	60.033	55.936	30.324	1.00 23.51	. C
MOTA	1315	CG1	ILE	Α	292	60.898	54.703	30.594	1.00 23.67	, C
MOTA	1316	CG2	ILE	A	292	58.561	55.563	30.426	1.00 23.40	C
MOTA	1317	CD1	ILE	Α	292	62.342	55.009	30.958	1.00 23.64	. C
MOTA	1318	N	VAL	A	293	61.823	58.393	29.481	1.00 23.36	N
MOTA	1319	CA	VAL	Α	293	63.084	59.137	29.478	1.00 23.68	C
MOTA	1320	C	VAL	Α	293	63.490	59.686	30.844	1.00 24.18	C
MOTA	1321	0	VAL	Α	293	64.459	60.439	30.946	1.00 24.31	. 0
ATOM	1322	CB	VAL	Α	293	63.033	60.329	28.480	1.00 23.27	C
ATOM	1323	CG1	JAV	Α	293	62.966	59.815	27.047	1.00 22.91	. С
ATOM	1324	CG2	VAL	A	293	61.823	61.209	28.776	1.00 22.79	C
MOTA	1325	N	ASP			62.750	59.328	31.889	1.00 24.54	
MOTA	1326	CA	ASP	Α	294	63.095	59.794	33.227	1.00 25.28	
MOTA	1327	С	ASP	Α	294	62.808	58.743	34.300	1.00 25.54	
MOTA	1328	0	ASP			62.245	57.688	34.013	1.00 25.69	
MOTA	1329	СВ	ASP			62.372	61.120	33.544	1.00 24.98	
MOTA	1330	CG	ASP			60.862	60.962	33.726	1.00 25.49	
ATOM	1331		ASP			60.290	59.921	33.347	1.00 26.22	
MOTA	1332		ASP			60.238	61.911	34.244	1.00 25.60	
ATOM	1333	N	GLY			63.221	59.031	35.531	1.00 26.27	
MOTA	1334	CA	GLY			63.008	58.106	36.628	1.00 26.98	
MOTA	1335.	C			295	61.553	57.787	36.914	1.00 27.45	
ATOM	1336	Ō	GLY			61.216	56.643	37.216	1.00 27.19	
ATOM	1337	N	GLU			60.686	58.793	36.829	1.00 28.15	
MOTA	1338	CA			296	59.263	58.582	37.084	1.00 29.28	
ATOM	1339	C.			296	58.669	57.578	36.110	1.00 28.28	
ATOM	1340	ō			296	57.908	56.705	36.508	1.00 28.87	
ATOM	1341	CB	GLU			58.477	59.889	36.959	1.00 31.29	
ATOM	1342	CG	GLU			58.771	60.920	38.014	1.00 35.34	
MOTA	1343	CD			296	57.900	62.166	37.866	1.00 38.57	
ATOM	1344		GLU					38.544	1.00 40.66	
ATOM	1344		GLU			58.213 56.910	63.169 62.148	37.081	1.00 40.66	
ATOM	1345	N N			297	58.996	57.728	34.830	1.00 33.46	
ATOM	1347	CA			297	58.482	56.819	33.821	1.00 27.33	
ATOM	1347	CA			297	58.997	55.406	34.032	1.00 26.40	
ATOM	1348	0			297	58.261	54.436	33.850	1.00 26.39	
111 011	エンセン	0	THE	_	231	JU.201	77.470	JJ.650	1.00 20.33	, 0

MOTA	1350	N	PHE	A	298	60.270	55.292	34.399	1.00	25.90		N
ATOM	1351	CA	PHE	Α	298	60.886	53.992	34.667	1.00	25.89		C
ATOM	1352	С			298	60.156	53.324	35.825	1.00	26.26	•	С
ATOM	1353	0			298	59.741	52.173	35.736		26.46		0
ATOM	1354	СВ			298	62.356	54.158	35.073		24.63		C
ATOM	1355	CG			298	62.973	52.900	35.625		24.52		C
ATOM	1356		PHE			63.510	51.935	34.774		24.45		C
ATOM	1357		PHE			62.948	52.642	36.993		24.69	•	C
MOTA	1358		PHE			64.004	50.729	35.283		24.11		C
MOTA	1359		PHE			63.438	51.441	37.506		24.45		C
MOTA	1360	CZ		•	298	63.965	50.485	36.648		24.01		С
ATOM	1361	N			299	60.038	54.071	36.917		26.97		N
MOTA	1362	CA	ARG	Α	299	59.392	53.627	38.148	1.00	27.76		C
MOTA	1363	С	ARG	А	299	57.979	53.112	37.896	1.00	27.50		C
MOTA	1364	0	ARG	Α	299	57.575	52.073	38.432	1.00	27.02		0
ATOM	1365	CB	ARG	A	299	59.368	54.798	39.134	1.00	29.28		С
MOTA	1366	CG	ARG	Α	299	58.488	54.625	40.354	1.00	32.58		C
ATOM	1367	CD	ARG	Α	299	59.185	53.881	41.472	1.00	34.72		C
ATOM	1368	NE			299	60.450	54.500	41.869	1.00	36.94		N
MOTA	1369	CZ			299	61.175	54.093	42.911		37.49		C
ATOM	1370		ARG			60.748	53.081	43.656		37.79		N
MOTA	1371	NH2	ARG			62.336	54.671	43.191	-	37.51		N
MOTA	1372	N			300	57.228	53.840	37.076		26.42		N
ATOM	1373	CA			300	55.867	53.448	36.764		26.07		C
MOTA	1374	C			300	55.807	52.106	36.028		25.82		C
ATOM	1375	0			300	54.967	51.263	36.332		25.66		0
MOTA	1376	CB			300	55,194	54.517	35.905		26.47		C
ATOM	1377	CG			300	53.740	54.220	35.612		26.10		C
MOTA	1378	CD1			300	52.755	54.430	36.583		25.70		С
ATOM	1379	CD2			300	53.349	53.726	34.367	1.00	25.87		C
ATOM	1380	CE1	TYR	Α	300	51.413	54.157	36.318	1.00	25.69		C
MOTA	1381	CE2	TYR	Α	300	52.013	53.450	34.092	1.00	26.08		C
MOTA	1382	CZ	TYR	Α	300	51.052	53.671	35.069	1.00	26.05		C
ATOM	1383	OH	TYR	Α	300	49.729	53.428	34.780	1.00	26.67		0
ATOM	1384	N			301	56687	51.912	35.054	1.00	24.94		N
ATOM	1385	CA	LEU	Α	301	56.686	50.667	34.297	1.00	24.79		С
ATOM	1386	С			301	57.290	49.516	35.104		25.13		С
ATOM	1387	Ō			301	56.933	48.356	34.910		24.72		0
ATOM	1388	СВ			301	57.422	50.860	32.965		23.46		C
ATOM	1389	CG			301	56.676	51.797	31.998		22.90		C
ATOM	1390				301	57.460	51.938	30.687		21.27		C
ATOM	1391		LEU			55.273	51.237	31.726		22.01		C
							49.844	36.020		25.45		N
ATOM	1392	N			302	58.194						
ATOM	1393	CA			302	58.803	48.828	36.867		.26.43		C
ATOM	1394	C			302	57.718	48.269	37.802		27.00		C
ATOM	1395	0			302	57.551	47.053	37.912		26.60		0
MOTA	1396	CB			302	59.944	49.433	37.676		25.79		С
MOTA	1397	N			303	56.976	49.163	38.456		27.78		N
MOTA	1398	CA			303	55.911	48.748	39.366		28.82		C
MOTA	1399	C			303	54.817	48.007	38.606		29.16		С
MOTA	1400	0	ASP	A	303	54.177	47.115	39.157	1.00	30.06		0
MOTA	1401	CB	ASP	. <b>A</b>	303	55.287	49.948	40.100	1.00	29.58		С
MOTA	1402	CG	ASP	А	303	56.218	50.565	41.138	1.00	31.14		С
MOTA	1403	OD1	ASP			57.081	49.848	41.693		31.95	-	0
MOTA	1404		ASP			56.070	51.774	41.417		32.16		0
MOTA	1405	N			304	54.594	48.382	37.348		28.83		N
ATOM	1406	CA			304	53.581	47.721	36.531		28.20		C
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MOTA	1407	С	ALA	A	304	54.008	46.288	36.197	1.00 28.33		С
MOTA	1408	0	ALA	A	304	53.179	45.461	35.818	1.00 28.02		0
MOTA	1409	CB	ALA	А	304	53.343	48.499	35.260	1.00 27.85	-	C
ATOM	1410	N	GLY	A	305	55.303	46.001	36.316	1.00 28.12		N
ATOM	1411	CA	GLY	A	305	55.777	44.649	36.051	1.00 27.69		С
MOTA	1412	C	GLY	A	305	56.626	44.386	34.820	1.00 27.36		С
MOTA	1413	0	GLY	A	305	56.891	43.228	34.486	1.00 27.45		0
MOTA	1414	N	ALA	Α	306	57.064	45.439	34.141	1.00 26.93		N
ATOM	1415	CA	ALA	А	306	57.884	45.268	32.945	1.00 26.72		C
ATOM	1416	C	ALA	A	306	59.144	44.438	33.220	1.00 26.12		С
MOTA	1417	0	ALA	A	306	59.759	44.557	34.277	1.00 26.19		0
MOTA	1418	CB	ALA	Α	306	58.271	46.642	32.382	1.00 26.69		С
MOTA	1419	N	ASP	Α	307	59.521	43.595	32.263	1.00 26.12		N
MOTA	1420	CA	ASP	Α	307	60.716	42.763	32.392	1.00 25.75		C
ATOM	1421	С	ASP	Α	307	61.976	43.541	31.989	1.00 25.56		С
MOTA	1422	0	ASP	Α	307	63.084	43.221	32.414	1.00 25.02		0
MOTA	1423	CB	ASP	Α	307	60.550	41.494	31.556	1.00 25.88		C
MOTA	1424	CG	ASP	Α	307	59.605	40.503	32.210	1.00 26.34		C
MOTA	1425	OD1	ASP			59.941	40.031	33.316	1.00 25.65		0
ATOM	1426	OD2	ASP	Α	307	58.532	40.208	31.639	1.00 26.39		0
MOTA	1427	N			308	61.791	44.553	31.148	1.00 25.21		N
ATOM	1428	CA			308·	62.872	45.435	30.739	1.00 25.37		С
MOTA	1429	С			308	62.207	46.715	30.251	1.00 25.54		С
ATOM	1430	0			308	61.096	46.689	29.718	1.00 26.05		0
ATOM	1431	·CB			308	63.803	44.781	29.692	1.00 24.85		C
ATOM	1432	CG			308	63.254	44.722	28,286	1.00 25.59		С
ATOM	1433		PHE			63.202	45.866	27.488	1.00 25.36		C
MOTA	1434	CD2	PHE			62.863	43.499	27.730	1.00 25.52		C
ATOM	1435		PHE			62.776	45.789	26.158	1.00 25.87		C
MOTA	1436	CE2	PHE			62.435	43.413	26.397	1.00 25.33		C
ATOM	1437	CZ			308	62.393	44.558	25.611	1.00 25.03		C
ATOM	1438	N			309	62.860	47.844	30.490	1.00 25.29		N
MOTA	1439	CA			309	62.293	49.126	30.118	1.00 25.21		C
ATOM	1440	. C			309	63.119	49.820	29.041	1.00.24.80		C
MOTA	1441	Ō			309	64.338	49.945	29.152	1.00 24.39		0
ATOM	1442	СВ			309	62.124	50.001	31.390	1.00 25.06		C
ATOM	1443	CG1			309	61.045	49.356	32.280	1.00 24.71		C
MOTA	1444	CG2	ILE			61.743	51.429	31.018	1.00 24.45		c
ATOM	1445		ILE			60.990	49.849	33.715	1.00 23.70		C
ATOM	1446	N			310	62.430	50.249	27.988	1.00 24.64		N
ATOM	1447	CA				63.066		26.850			C
ATOM	1448	C			310	63.134	52.416	27.024	1.00 24.46		C
MOTA	1449	Ō			310	62.146	53.060	27.373	1.00 24.21		Ō
MOTA	1450	СВ			310	62.311	50.509	25.574	1.00 25.07		C
MOTA	1451	CG			310	63.177	50.404	24.340	1.00 25.07		C
MOTA	1452	CD	LYS			62.769	49.218	23.461	1.00 25.06		Ċ
ATOM	1453	CE			310	61.376	49.398	22.850	1.00 25.52		Č
ATOM	1454	NZ			310	61.267	50.678	22.090	1.00 25.01		N
ATOM	1455	N			311	64.316	52.971	26.768	1.00 24.00		N
ATOM	1456	CA			311	64.571	54.401	26.925	1.00 23.52		C
ATOM	1457	C			311	64.715	55.166	25.613	1.00 23.91		C
ATOM	1458	Õ			311	65.486	54.776	24.737	1.00 23.10		0
ATOM	1459	CB			311	65.883	54.643	27.715	1.00 22.79		C
ATOM	1460		ILE			65.828	53.933	29.070	1.00 22.26		C
ATOM	1461		ILE			66.121	56.146	27.878	1.00 21.49		C
ATOM	1462		ILE			67.200	53.802	29.751	1.00 21.78		C
ATOM	1463	N			312	63.991	56.270	25.484	1.00 24.94	• •	N
							30.0.0				

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MOTA	1464	CA	GLY				64.137	57.058	24.280		26.52			С
ATOM	1465	C	$\operatorname{GLY}$	Α	312		62.921	57.644	23.599		28.07			C
MOTA	1466	0	GLY	Α	312		62.052	56.925	23.108	1.00	27.43			0
ATOM	1467	N	ILE	A	313		62.876	58.971	23.575	1.00	30.06			N
ATOM	1468	CA	ILE	A	313		61.819	59.715	22.907	1.00	32.43			С
MOTA	1469	C	ILE	Α	313		62.497	60.917	22.262	1.00	34.74			С
MOTA	1470	0	ILE				63.031	61.788	22.954	1.00	33.88			0
MOTA	1471	СВ	ILE				60.745	60.229	23.881		32.08			С
ATOM	1472	CG1	ILE				60.029	59.055	24.554		31.93			C
ATOM	1473		ILE				59.735	61.071	23.117		32.14			C
ATOM	1474.		ILE				58.970	59.481	25.560		31.83			C
ATOM	1475	N	GLY				62.484	60.959	20.935		37.68			N
		CA												C
ATOM	1476		GLY				63.115	62.065	20.241		41.68			
MOTA	1477	C	GLY				64.614	61.848	20.205		44.77			C
ATOM		0	GLY				65.380	62.540	20.898		45.22			0
ATOM	1479	N .	GLY				65.025	60.864	19.406		46.78	-	•	N
MOTA	1480	CA	GLY				66.432	60.539	19.265		49.14			С
MOTA	1481	С	GLY				66.702	59.826	17.952		50.80			С
MOTA	1482	0	GLY	Α	315		67.732	60.057	17.310	1.00	51.20			0
ATOM	14.83	N	GĻY	Α	316	. '	65.774	58.962	17.547	1.00	52.08			N
ATOM	1484	CA	GLY	Α	316		65.934	58.224	16.304	1.00	53.45			С
MOTA	1485	C	GLY	A	316		66.265	59.085	15.092	1.00	54.43			С
ATOM	1486	0	GLY	A	316		66.109	60.310	15.124	1.,00	54.52			0
MOTA	1487	N	SER	Α	317·	•	66.718	58.437	14.019	1.00	55.17			N
ATOM	1488	CA	SER	А	317		67.086	59.120	12.776	1.00	55.85			C
ATOM	1489	С			317		66.116	60.238	12.410	1.00	56.05			С
ATOM	1490	0			317		66.224	60.838	11.338		56.24			0
ATOM	1491	СВ			317		67.152	58.117	11.618		56.06			C
ATOM	1492	OG			317		68.116	57.109	11.864		56.47			0
ATOM.	1493	N	ARG				60.666	65.002	18.046		69.94			N
ATOM	1494	CA	ARG				60.632	66.036	19.075		69.88			C
ATOM	1495	C	ARG				60.442	67.421	18.458		69.25			C
ATOM	1496		ARG					68.357	19.123		69.33			0
		O _.					59.992							
ATOM	1497	CB	ARG				61.922	65.990	19.904		70.76			C
ATOM	1498	CG	ARG				63.200	66.013	19.077		72.26			C
ATOM	1499	CD	ARG				64.412	65.622	19.916		73.59			C
ATOM	1500	NE	ARG				65.616	65.472	19.098		75.09			Ŋ
MOTA	1501		-ARG				66.295	66.483	18.561		75.74			С
MOTA	1502		ARG				65.893	67.733	18.757		75.89			N
MOTA		NH2	ARG				67.372	66.241	17.818		75.84			N
MOTA	1504	N	GLU	A	323		60.786	67.544	17.180	1.00	68.34			N
ATOM	1505	CA	GLU				60.638	68.805	16.466	1.00	66.98			С
MOTA	1506	С			323		59.314	68.796	15.706	1.00	65.40			C
MOTA	1507	0	GLU	Α	323		59.205	69.339	14.603	1.00	65.33	•		0
MOTA	1508	CB	GLU	Α	323		61.805	69.003	15.495	1.00	68.07			С
MOTA	1509	CG	GLU	Α	323 .		63.168	69.072	16.178	1.00	69.20			С
ATOM	1510	CD	GLU	А	323		64.322	69.148	15.188	1.00	70.01			С
MÓTA	1511	OE1	GLU	A	323		64.371	70.116	14.393	1.00	70.24			0
MOTA	1512	OE2					65.181	68.238	15.209		70.24			0
ATOM	1513	N.			324		58.311	68.163	16.311		63.21			N
ATOM	1514	CA	GLN				56.982	68.075	15.722		60.76			C
ATOM	1515	C			324		55.916	68.047	16.814		58.40			C
ATOM	1516	0	GLN				54.859	68.662	16.679		58.63			0
ATOM	1517	CB	.GTM				56.861	66.821	14.852		61.63	•		C
ATOM	1518	CG			324		55.533	66.714	14.120		62.44			C
ATOM	1519	CD			324		55.341	67.814	13.085		63.06			C
ATOM	1520								13.363		63.40			0
ATOM	1240	OET	GLN	н	J 2 4		55.567	68.996	13.303	1.00	05.40			J

MOTA	1521	NE2	GLN	Ά	324	54.910	67.431	11.887	1.00	63.02		N
MOTA	1522	N	LYS	Α	325	56.193	67.329	17.897	1.00	55.16		N
ATOM.	1523	CA	LYS	A	325	55.246	67.250	19.001	1.00	51.62		C
MOTA	1524	C	LYS	Α	325	55.822	67.983	20.207	1.00	48.73		C
MOTA	1525	0	LYS	Α	325	55.092	68.412	21.099	1.00	48.29	,	0
ATOM	1526	CB	LYS	A	325	54.962	65.789	19.347	100	52.41		C
ATOM	1527	CG	LYS			53.645	65.576	20.063		52.70		С
MOTA	1528	CD	LYS			53.291	64.104	20.115		53.01		С
ATOM	1529	CE			325	51.906	63.905	20.678		53.28		C
ATOM	1530	NZ			325	51.527	62.469	20.681		54.05		N
ATOM	1531	N	GLY			57.141	.68.124	20.225		45.49		N
ATOM	1532	CA	GLY			57.789	68.832	21.311		42.06		C
ATOM	1533	C			326	58.097	68.028	22.558		39.58		C
ATOM	1534	0	GLY			58.407	68.613	23.591		38.74		0
ATOM	1535	N			327	58.002	66.703	22.478		37.33		N
	1536	CA								35.54		C
ATOM					327	58.302	65.861	23.629				
ATOM	1537	C			327	59.598	65.096	23.385		34.11		C
ATOM	1538	0			327	59.911	64.723	22.256	*	33.94		0
ATOM	1539	CB			327	57.165	64.836	23.936		35.64		C
ATOM	1540	CG1	ILE			57.042	63.815	22.807		35.72		C
ATOM	1541	CG2			327	55.837	65.563	24.130		35.90		C
ATOM	1542	CD1	ILE			56.106	62.650	23.131		36.15		C
MOTA	1543	N			328	60.357	64.869	24.447		32.52		N
ATOM	1544	CA			328	61.599	64.142	24.295		30.76		С
MOTA	1545	C			328	62.680	64.581	25.260		29.34		С
MOTA	1546	0	GLY	А	328	62.447	65.403	26.153	1.00	27.81		0
MOTA	1547	N	ARG	Α	329	63.874	64.030	25.066	1.00	27.97		N
MOTA	1548	CA	ARG	Α	329	65.008	64.343	25.919	1.00	27.02		C
MOTA	1549	C	ARG	A	329	66.265	63.793	25.272	1.00	26.17		С
MOTA	1550	0	ARG	Α	329	66.222	62.730	24.657	1.00	26.57		0
MOTA	1551	CB	ARG	Α	329	64.813	63:691	27.295	1.00	26.66		C
ATOM	1552	CG	ARG	Α	329	65.752	64.198	28.374	1.00	25.97		С
ATOM	1553	CD			329	65.514	63.470	29.688		26.09		С
MOTA	1554	NE	ARG			65.797	64.324	30.835		26.17		N
MOTA	1555	CZ	ARG			65.626	63.964	32.103		27.08		C
ATOM	1556		ARG			65.177	62.752	32.408		26.65		N
ATOM	1557		ARG			65.884	64.829	33.072		27.28		N
ATOM	1558	N	GLY			67.377	64.513	25.396		25.55		N
ATOM	1559	CA	GLY			68.625	64.021	24.837		24.59		C
ATOM	1560	C	GLY			68.797	62.587	25.311		24.12		C
ATOM	1561	0	GLY			68.580	62.287	26.482		23.28		0
ATOM	1562	N			331	69.180	61.698	24.404		24.45		N
ATOM	1563	CA			331	69.332	60.286	24.729		24.31		C
MOTA	1564	C						25.883				C
		0			331	70.295	60.017			24.63 24.51		
ATOM	1565 1566				331	70.000	59.191	26.751				0
ATOM		CB			331	69.772	59.505	23.486		24.66		C
ATOM	1567	CG			331	69.635	57.989	23.627		25.35		C
ATOM	1568	CD			331	68.181	57.536	23.753		26.40		C
ATOM	1569		GLN			67.905	56.422	24.197		27.18		0
ATOM	1570	NE2				67.251	58.395	23.351		25.73		N
ATOM	1571	N			332	71.435	60.713	25.904		23.94		N
MOTA	1572	CA			332	72.420	60.515	26.964		23.57		C
MOTA	1573	С			332	71.833	60.835	28.338		23.62		C
MOTA	1574	0			332	71.955	60.044	29.278		23.57		0
ATOM	1575	CB			332	73.669	61.375	26.702	1.00	23.41		С
MOTA	1576	N			333	71.192	61.993	28.451	1.00	23.21		N
ATOM	1577	CA	THR	A	333	70.584	62.403	29.707	1.00	22.90		C

ATOM	1578	С	THR	Α	333	69.500	61,408	30.105	1.00	23.18		С
MOTA	1579	0	THR	Α	333	69.380	61.031	31.273	1.00	22.90		0
MOTA	1580	CB	THR	Α	333	69.967	63.814	29.590	1.00	22.97		С
ATOM	1581	OG1	THR	A	333	70.992	64.751	29.222	1.00	22.52		0
MOTA	1582	CG2	THR	Α	333	69.349	64.240	30.922	1.00	21.69		С
MOTA	1583	N	ALA	Α	334	68.717	60.977	29.123		23.07		N
MOTA	1584	CA	ALA			67.648	60.018	29.373		23.70	•	С
MOTA	1585	C.	ALA			68.206	58.718	29.963		23.40		С
ATOM	1586	0	ALA			67.717	58.223	30.977		23.84		0
ATOM	1587	СВ	ALA			66.890	59.731	28.070		23.17		C
ATOM	1588	N	VAL			69.231	58.168	29.324		23.69		N
ATOM	1589	CA	VAL			69.842	56.933	29.797		24.02		C
ATOM	1590	C	VAL			70.430	57.107	31.194		24.09		C
ATOM	1591	0	VAL			70.430	56.316	32.100		24.31		0
MOTA	1592	CB	VAL			70.147	56.459	28.837		24.63		C
ATOM	1593		VAL			71.682	55.254	29.431		25.02		c
												C
ATOM	1594					70.348	56.090	27.487		24.84		
ATOM	1595	N	ILE			71.240	58.147	31.371		24.11		N
ATOM	1596	CA	ILE			71.867	58.416	32.661		23.87		C
MOTA	1597	C	ILE			70.851	58.544	33.801		24.46		C
ATOM	1598	0	ILE			71.039	57.963	34.874		23.73		0
MOTA	1599	CB	ILE			72.725	59.701	32.607		23.35		C
ATOM	1600	CG1	ILE			73.913	59.495	31.660		22.68		C
MOTA	1601	CG2	ILE	Α	336	73.234	60.055	34.008		22.89		C
ATOM	1602	CD1	ILE	Α	336	74.743	60.756	31.431		22.49		C
MOTA	1603	N	ASP	Α	337	69.775	59.296	33.572	1.00	24.98		N
ATOM	1604	CA ·	ASP	А	337	68.759	59.479	34.606	1.00	25.52		C
MOTA	1605	С	ASP	Α	337	67.938	58.219	34.875	1.00	24.84		С
MOTA	1606	0	ASP	Α	337	67.629	57.907	36.024	1.00	24.56		0
ATOM	1607	CB	ASP	Α	337	67.818	60.637	34.245	1.00	27.31		C
ATOM	1608	CG	ASP	Α	337	68.502	62.000	34.327	1.00	30.71		C
MOTA	1609	OD1	ASP	A	337	69.614	62.096	34.913	1.00	32.05		0
ATOM	1610		ASP			67.918	62.983	33.815		31.24		0
MOTA	1611	N	VAL			67.569	57.501	33.822	1.00	24.57		N
ATOM	1612	CA	VAL			66.787	56.280	34.006		23.99		C
ATOM	1613	C	VAL			67.631	55.230	34.735		23.85		C
ATOM	1614	0	VAL			67.139	54.547	35.627		23.32		0
ATOM	1615	СВ	VAL			66.288	55.716	32.646		23.60		C
ATOM	1616	CG1	VAL			65.631	54.347	32.848		23.15		C
ATOM	1617	CG2	VAL			65.280	56.690	32.019		22.47		C
MOTA	1618	N	VAL			68.906	55.126	34.362		23.84		
			VAL									N
ATOM	1619	CA				69.816	54.165	34.981		24.21		C
ATOM	1620	C	VAL			69.980	54.429	36.480		25.13		C
ATOM	1621	0	VAL			70.043	53.493	37.278		25.49		0
ATOM	1622	CB	VAL			71.215	54.195	34.289		23.92		C
ATOM	1623		VAL			72.270	53.502	35.158		23.40		C
MOTA	1624		VAL			71.134	53.503	32.940		23.43		C
ATOM	1625	N	ALA			70.053	55.700	36.866		25.88		N
MOTA	1626	CA	ALA			70.202	56.042	38.278		26.36		С
MOTA	1627	С	ALA			68.959	55.600	39.051		26.83		С
MOTA	1628	0	ALA			69.053	55.132	40.185		26.86		0
MOTA	1629	CB	ALA	Α	340	70.419	57.540	38.437		26.17		С
MOTA	1630	N	GLU			67.796	55.750	38.429	1.00	27.07		N
MOTA	1631	CA	GLU			66.542	55.358	39.061	1.00	27.92		C
MOTA	1632	С	GLU			66.472	53.834	39.131	1.00	27.70		C
MOTA	1633	0	GLU	A	341	66.016	53.273	40.124	1.00	27.73		0
MOTA	1634	CB	GLU	A	341	65.358	55.898	38.256	1.00	28.93		С
	•											

ATOM	1635	CG	GLU	A	341	64.004	55.796	38.960	1.00 30.89	C
MOTA	1636	CD	GLU	A	341	63.955	56.592	40.258	1.00 32.66	C
MOTA	1637	OE1	GLU	Α	341	64.480	57.727	40.299	1.00 34.48	0
ATOM	1638	OE2	GLU	A	341	63.380	56.090	41.240	1.00 34.06	0
MOTA	1639	N	ARG	A	342	66.926	53.173	38.067	1.00 27.14	N
MOTA	1640	CA	ARG	Α	342	66.928	51.714	37.999	1.00 26.71	C
MOTA	1641	C	ARG	Α	342	67.821	51.149	39.103	1.00 26.54	C
MOTA	1642	0	ARG	Α	342	67.497	50.130	39.716	1.00 26.18	0
ATOM	1643	СВ	ARG	A	342	67.426	51.254	36.618	1.00 25.95	C
ATOM	1644	CG	ARG			67.409	49.739	36.373	1.00 24.78	C
MOTA	1645	CD	ARG			68.642	49.033	36.940	1.00 23.69	С
MOTA	1646	NE	ARG	Α	342	69.905	49.458	36.335	1.00 23.29	N
MOTA	1647	CZ	ARG	A	342	70.262	49.229	35.070	1.00 23.19	С
MOTA	1648	NH1	ARG			69.453	48.574	34.247	1.00 22.48	И
ATOM	1649	NH2	ARG			71.442	49.648	34.626	1.00 22.80	N
ATOM	1650	N	ASN			68.943	51.815	39.354	1.00 26.63	N
MOTA	1651	CA	ASN			69.866	51.363	40.389	1.00 27.25	С
MOTA	1652	С	ASN			69.271	51.619	41.770	1.00 28.00	С
MOTA	1653	0	ASN	Α	343	69.415	50.804	42.680	1.00 27.55	. 0
ATOM	1654	CB	ASN	А	343	71.222	52.055	40.238	1.00 26.44	C
ATOM	1655	CG	ASN			71.979	51.575	39.008	1.00 26.67	C
MOTA	1656	OD1	ASN	A	343	71.660	50.523	38.445	1.00 26.42	0
MOTA	1657	ND2	ASN	Α	343	72.995	52.330	38.595	1.00 25.68	N
MOTA	1658	N	LYS	Α	344	68.585	52.748	41.913	1.00 28.63	N
MOTA	1659	CA	LYS	A	344	67.937	53.089	43.168	1.00 30.19	C
ATOM	1660	C	LYS	Α	344	66.852	52.044	43.419	1.00 30.06	C,
MOTA	1661	0	LYS	Α	344	66.702	51.536	44.530	1.00 30.48	0
MOTA	1662	CB	LYS	А	344	67.308	54.481	43.073	1.00 31.64	С
MOTA	1663	CG	LYS	A	344	66.560	54.917	44.323	1.00 34.82	C
MOTA	1664	CD	LYS	Α	344	65.887	56.276	44.143	1.00 36.84	C
ATOM	1665	CE	LYS	A	344	66.890	57.354	43.756	1.00 38.89	C
MOTA	1666	NZ	LYS	А	344	66.248	58.707	43.638	1.00 41.17	N
MOTA	1667	N	TYR	Α	345	66.107	51.723	42.367	1.00 29.84	N
MOTA	1668	CA	TYR	A	345	65.032	50.743	.42.443	1.00 30.10	C
MOTA	1669	С	TYR	A	345	65.576	49.370	42.854	1.00 30.60	C
ATOM	1670	0	TYR	Α	345	64.960	48.665	43.654	1.00 30.17	0
ATOM	1671	CB	TYR	Α	345	64.334	50.635	41.088	1.00 29.60	C
MOTA	1672	CG	TYR	A	345	63.051	49.828	41.103	1.00 30.01	C
MOTA	1673	CD1	TYR	Α	345	61.847	50.407	41.508	1.00 29.92	C
MOTA	1674	CD2	TYR	Α	345	63.032	48.499	40.675	1.00 29.79	C
MOTA	1675	CE1	TYR	Α	34Š	60.658	49.690	41.476	1.00 30.21	C
ATOM	1676	CE2	TYR	Α	345	61.843	47.770	40.641	1.00 30.08	C
MOTA	1677	CZ	TYR	Α	345	60.662	48.376	41.040	1.00 30.51	C
MOTA	1678	OH	TYR	A	345	59.479	47.685	40.978	1.00 31.68	0
MOTA	1679	N	PHE	Α	346	66.726	48.996	42.298	1.00 31.26	N
ATOM	1680	CA	PHE	Α	346	67.351	47.717	42.619	1.00 32.37	C
ATOM	1681	C	PHE	Α	346	67.722	47.651	44.102	1.00 33.09	C
ATOM	1682	0	PHE	A	346	67.528	46.630	44.754	1.00 32.99	0
MOTA	1683.	CB	PHE	Α	346	68.613	47.509	41.781	1.00 32.81	C.
MOTA	1684	CG	PHE	Α	346	69.374	46.269	42.141	1.00 33.53	С
ATOM	1685	CD1	PHE	Α	346	68.841	45.011	41.881	1.00 33.63	С
ATOM	1686	CD2	PHE	A	346	70.608	46.357	42.777	1.00 34.62	C
ATOM	1687	CE1	PHE	A	346	69.519	43.858	42.246	1.00 34.10	С
ATOM	1688	CE2	PHE	A	346	71.301	45.206	43.152	1.00 35.41	C
ATOM	1689	CZ			346	70.750	43.950	42.883	1.00 35.25	С
ATOM	1690	N			347	68.260	48.745	44.626	1.00 33.99	N
MOTA	1691	CA			347	68.646	48.803	46.026	1.00 35.45	С

ATOM	1692	С	GLU				67.435	48.732	46.958	1.00	35.29			С
ATOM	1693	0	GLU	Α	347		67.540	48.231	48.075	1.00	35.27			0
ATOM	1694	CB	GLU	A	347		69.429	50.088	46.312	1.00	36.72			С
MOTA	1695	CG	GLU	A	347		70.769	50.204	45.594	1.00	40.50			С
ATOM	1696	CD	GLU	A	347		71.714	49.039	45.888	1.00	42.72			С
MOTA	1697	OE1	GLU	A	347		71.826	48.625	47.069	1.00	44.09			0
MOTA	1698	OE2	GLU	A	347		72.360	48.544	44.935	1.00	44.09			0
MOTA	1699	N	GLU	Α	348		66.287	49.225	46.504	1.00	35.07			N
MOTA	1700	CA	GLU	Α	348		65.089	49.221	47.337	1.00	35.42			С
ATOM	1701	С	GLU				64.306	47.914	47.303		34.55			C
ATOM	1702	0	GLU				63.739	47.502	48.309	1.00	34.49			0
MOTA	1703	CB	GLU				64.127	50.339	46.915	•	37.00			C
ATOM	1704	CG	GLU				64.759	51.699	46.683		39.47			C
ATOM	1705	CD	GLU				63.750		46.194		40.68			Ċ
ATOM	1706	OE1	GLU				62.928	52.416	45.308		41.24			ō
ATOM	1707	OE2	GLU				63.788	53.883	46.690		41.95			ŏ
ATOM	1708	N	THR				64.281	47.266	46.143		33.77			N
ATOM	1709	CA	THR				63.501	46.049	45.957		32.68			C
ATOM	1710	C	THR				64.277	44.756	45.706		32.25			C
ATOM	1711	0	THR				63.717	43.670	45.813		32.24			0
							•				32.69			C
ATOM	1712	CB	THR				62.534	46.231	44.770					
ATOM	1713	OG1					63.296	46.372	43.562		32.06			0
ATOM	1714	CG2					61.678	47.481	44.959		32.19			C
MOTA	1715	N	GLY				65.554	44.867	45.363		31.82			И
ATOM	1716	CA	GLY				66.335	43.678	45.072		30.66			C
ATOM	1717	C	GLY				66.068	43.202	43.648		29.93			С
MOTA	1718	0	GLY			•	66.557	42.157	43.220		30.20			0
MOTA	1719	N	ILE				65.287	43.978	42.906		28.99			N
MOTA	1720	CA	ILE				64.950	43.633	41.529		27.61			С
MOTA	1721	C	ILE				65.773	44.447	40.538		26.84			С
MOTA	1722	0	ILE				65.744	45.675	40.558		26.06			0
MOTA	1723	CB	ILE				63.459	43.901	41.239	1.00	27.81			С
MOTA	1724	CG1	ILE				62.588	43.128	42.233	1.00	27.74			С
MOTA	1725	CG2	ILE	A	351		63.123	43.498	39.802	1.00	27.06			С
MOTA	1726	CD1	ILE	A	351		61.150	43.611	42.277	1.00	27.83			С
MOTA	1727	N	TYR	A	352 ू		66.518	43.757	39.681	1.00	26.12			N
MOTA	1728	CA	TYR	A	352		67.323	44.431	38.675	1.00	25.65			C
MOTA	1729	C	TYR	Α	352		66.570	44.364	37.358	1.00	25.14			С
MOTA	1730	0	TYR	Α	352	•	66.344	43.279	36.829	1.00	25.00			0
MOTA	1731	CB	TYR	Α	352		68.682	43.754	38.490	1.00	24.90			С
MOTA	1732	CG	TYR	Α	352		69.562	44.497	37.502	1.00	24.91			С
MOTA	1733	CD1	TYR	Α	352	٠.	70.365	45.561	37.915	1.00	24.55			С
MOTA	1734	CD2	TYR	A	352		69.574	44.150	36.152	1.00	24.86			С
ATOM	1735	CE1	TYR	Α	352		71.161	46.258	37.010	1.00	25.05			С
MOTA	1736	CE2	TYR	Α	352		70.371	44.843	35.234	1.00	24.70		,	С
	1737	CZ	TYR				71.161	45.892	35.670		24.84			C
MOTA	1738	ОН	TYR				71.976	46.555	34.783		24.66			0
ATOM	1739	N			353		66.181	45.522	36.835		25.14			N
ATOM	1740	CA	ILE				65.455	45.581	35.574		24.39			C
ATOM	1741	C			353		66.364	46.094	34.467		24.46			C
ATOM	1742	0			353		66.838	47.229	34.519		24.61			0
ATOM	1743	CB			353		64.234	46.515	35.678		25.03			C
ATOM	1744		ILE				63.298	46.017	36.786		24.96			C
ATOM	1745		ILE				63.499	46.567	34.336		24.60			C
ATOM	1745		ILE				62.097	46.889	37.009		25.74			C
ATOM	1747	N			354		66.635	45.256	33.453		24.02			N
ATOM	1747	CA												C
WI OIA	1/40	CA	UNI	H	354		67.504	45.700	32.356	1.00	23.55			C

ATOM	1749	C.	PRO	А	354	66.849	46.858	31.617	1.00	23.06		C
ATOM	1750	0	PRO	A	354	65.627	46.896	31.491	1.00	23.02		0
ATOM	1751	CB	PRO	A	354	67.619	44.454	31.470	1.00	23.02	•	С
ATOM	1752	CG	PRO			67.455	43.318	32.455	1.00	23.37		С
ATOM	1753	CD ·	PRO	A	354	66.323	43.819	33.334	1.00	23.29		C
ATOM	1754	N .	VAL			67.652	47.807	31.142	1.00	22.63		N
ATOM	1755	CA	VAL			67.107	48.929	30.398	1.00			C
MOTA	1756	C	VAL			67.732	48.959	29.011	1.00			С
ATOM	1757	0	VAL			68.885	48.573	28.817	1.00			0
MOTA	1758	CB	VAL			67.318	50.296	31.134	1.00			C
MOTA	1759		VAL			66.618	50.258	32.483	1.00			C
ATOM	1760		VAL			68.806	50.617	31.293	1.00			C
ATOM	1761	N	CYS			66.950	49.408	28.044	1.00			N
MOTA	1762	CA	CYS			67.394	49.457	26.667	1.00			C
ATOM	1763	C	CYS			67.484	50.882	26.130	1.00			Č
ATOM	1764	Ō	CYS			66.510	51.633	26.191	1.00			Ō
ATOM	1765	ĊB			356	66.422	48.643	25.801	1.00			Ċ
ATOM	1766	SG	CYS			66.671	48.801	24.017	1.00			s
ATOM	1767	N			357	68.657	51.255	25.621	1.00			N
	1768	CA			357	 68.819	52.577	25.021	1.00			C
ATOM	1769	C			357	68.312	52.425	23.601	1.00			C
ATOM	1770	0			357	68.930	51.746	22.783	1.00			0
ATOM	1771	CB			357	70.283	53.013	25.027	1.00			C
ATOM	1772	OG			357	70.283		24.490	1.00			0
ATOM	1773	N	ASP			67.177	53.051	23.315	1.00		•	И
ATOM	1774	CA					52.951	21.998	1.00			C
ATOM		CA	ASP		358	66.554	54.226		1.00			C
	1775				358	66.654	55.244	21.164	1.00			0
MOTA	1776	O				66.047		21.494	1.00			C
ATOM	1777	CB			358	65.081	52.549	22.182	1.00			C
MOTA	1778	CG			358	64.336	52.369	20.867				
MOTA	1779		ASP			64.978	52.209	19.804	1.00		,	0
ATOM	1780		ASP			63.088	52.369	20.909	1.00			0
MOTA	1781	N			359	67.427	54.151	20.083		27.42		N
MOTA	1782	CA			359	67.585	55.281	19.186	1.00			C
MOTA	1783	C			359	68.670	56.272	19.559	1.00			C
ATOM	1784	0			359	69.235	56.224	20.652	1.00			0
ATOM	1785	N			360	68.975	57.171	18.631	1.00			N
ATOM	1786	CA			360	69.983	58.183	18.883	1.00			C
ATOM	1787	C			360	71.415	57.733	18.679	1.00			C
ATOM	1788	0			360	72.343	58.451	19.049	1.00			0
ATOM	1789	N			361	71.611		18.105	1.00		•	N
ATOM	1790	CA			361	72.962	56.069	17.871	1.00			C
MOTA	1791	C			361	73.376	56.307	16.426	1.00			C
ATOM	1792	0			361	72.908	55.631	15.502	1.00			0
MOTA	1793	CB			361	73.100	54.572	18.249	1.00			C
ATOM	1794		ILE			73.124	54.459	19.783	1.00			C
ATOM	1795		ILE			74.344	53.961	17.601	1.00			C
	.1796		ILE			73.769	53.223	20.332	1.00			C
ATOM	1797	N			362	74.257	57.288	16.244	1.00			N
ATOM	1798	CA			362	74.746	57.655	14.924	1.00			C
ATOM	1799	C			362	76.048	56.942	14.566	1.00		-	C
ATOM	1800	0			362	76.193	56.430	13.455	1.00			0
ATOM	1801	CB			362	74.973	59.179	14.829	1.00			C
ATOM	1802		VAL			75.272	59.577	13.386		42.28		C
ATOM	1803		VAL			73.751	59.916	15.347		42.45		C
ATOM	1804	N			363	76.987	56.902	15.510	1.00			N
ATOM	1805	CA	TYR	A	363	78.282	56.260	15.283	1.00	40.38		С

MOTA	1806	С	TYR	A	363	78.523	55.080	16.219	1.00 39.29	С
ATOM	1807	0	TYR	А	363	77.904	54.985	17.278	1.00 38.90	0
MOTA	1808	CB	TYR	Α	363	79.396	57.293	15.454	1.00 41.48	C
MOTA	1809	CG	TYR	Α	363	79.233	58.478	14.535	1.00 43.32	С
ATOM	1810-	CD1	TYR	A	363	79.265	58.315	13.150	1.00 44.27	С
MOTA	1811	CD2	TYR			79.001	59.755	15.045	1.00 44.05	· c
MOTA	1812	CE1	TYR	Α	363	79.067	59.392	12.293	1.00 45.45	С
ATOM	1813	CE2	TYR			78.801	60.841	14.197	1.00 45.25	C
ATOM	1814	CZ			363	78.836	60.652	12.822	1.00 45.68	c
ATOM	1815	OH			363	78.647	61.719	11.972	1.00 47.00	Ō
MOTA	1816	N	ASP			79.425	54.182	15.828	1.00 37.99	. <b>N</b>
ATOM	1817	CA	ASP			79.731	53.016	16.649	1.00 36.91	c
ATOM	1818	C	ASP			80.088	53.368	18.089	1.00 35.76	c
ATOM	1819	0	ASP			79.629	52.701	19.018	1.00 35.70	0
ATOM	1820	CB	ASP			80.892	52.701	16.062	1.00 37.35	c
	1821	CG	ASP							
MOTA						80.504	51.412	14.824	1.00 37.70	C
ATOM	1822		ASP			79.312	51.080	14.647	1.00 37.53	0
ATOM	1823		ASP			81.417	51.102	14.033	1.00 38.32	0
MOTA	1824	N				80.898	54.407	18.283	1.00,34.01	N
MOTA	1825	CA			365	81.304	54.771	19.638	1.00 33.07	C
MOTA	1826	С			365	80.131	55.199	20.524	1.00 31.99	C
MOTA	1827	0			365	80.255	55.228	21.745	1.00 31.66	0
MOTA	1828	CB	TYR			82.413	55.840	19.609	1.00 32.88	С
MOTA	1829	CG	TYR	Α	365	81.962	57.282	19.513	1.00 33.91	С
MOTA	1830	CD1	TYR	A	365	81.650	58.015	20.660	1.00 33.73	C
MOTA	1831	CD2	TYR	A	365	81.883	57.927	18.278	1.00 34.01	C
MOTA	1832	CEl	TYR	A	365	81.275	59.357	20.578	1.00 34.76	C
MOTA	1833	CE2	TYR	A	365	81.507	59.268	18.184	1.00 34.68	С
MOTA	1834	CZ	TYR	A	365	81.206	59.977	19.335	1.00 34.89	C
MOTA	1835	OH	TYR	A	365	80.841	61.302	19.239	1.00 35.48	0
ATOM	1836	N	HIS	Α	366	78.995	55.519	19.912	1.00 31.15	N
ATOM	1837	CA	HIS			77.807	55.886	20.680	1.00.30.50	C
MOTA	1838	С	HIS	A	366	77.305	54.640	21.411	1.00 29.58	C
ATOM	1839	0	HIS			76.639	54.742	22.439	1.00 28.57	0
MOTA	1840	CB	HIS			76.694	56.411	19.767	1.00 31.15	C
ATOM	1841	CG	HIS			76.918	57.806	19.275	1.00 32.03	, , C
ATOM	1842		HIS			77.928	58.613	19.753	1.00 32.57	N
ATOM	1843		HIS			76.227	58.557	18.383	1.00 32.25	C
MOTA	1844		HIS			77.848	59.800	19.179	1.00 32.26	, ç
ATOM	1845		HIS			76.824	59.793	18.346	the state of the s	, N
ATOM	1846	N			367	77.618	53.466	20.861	1.00 28.34	N
MOTA	1847	CA	MET			77.215	52.201	21.475	1.00 27.90	C
MOTA	1848	C	MET			77.213	52.050	22.801	1.00 26.79	C
ATOM	1849	0	MET			77.350	51.752	23.829	1.00 26.19	0
MOTA	1850	CB	MET					20.577	1.00 20.19	
					367	77.573	51.008			C
MOTA	1851	CG				76.771	50.894	19.285	1.00 28.28	C
MOTA	1852	SD	MET			77.371	49.505	18.270	1.00 29.89	S
MOTA	1853	CE			367	76.390	49.722	16.782	1.00 29.69	C
ATOM	1854	N			368	79.262	52.256	22.758	1.00 26.73	N
ATOM	1855	CA	THR			80.095	52.142	23.945	1.00 26.43	C
MOTA	1856	C			368	79.609	53,.141	24.993	1.00 26.11	C
MOTA	1857	0	THR			79.501	52.804	26.168	1.00 26.83	0
	1858	CB	THR			81.572	52.399	23.592	1.00 26.81	C
MOTA	1859		THR			81.911	51.638	22.424	1.00 26.87	0
MOTA	1860		THR			82.480	51.975	24.738	1.00 26.28	С
MOTA	1861	N			369	79.302	54.362	24.565	1.00 25.06	N
MOTA	1862	CA	LEU	Α	369	78.801	55.380	25.482	1.00 24.58	С

MOTA	1863	C	LEU	A	369	77.494	54.938	26.142	1.00 23.9	9	С
MOTA	1864	0	LEU	А	369	77.352	55.015	27.360	1.00 23.7	70	0
ATOM	1865	CB	LEU	A	369	78.567	56.706	24.744	1.00 24.3	31	C
ATOM	1866	CG	LEU	A	369	79.799	57.572	24.453	1.00 25.4	· 5	С
ATOM	1867	CD1	LEU	Α	369	79.369	58.829	23.700	1.00 24.6	53	C
ATOM	1868	CD2	LEU	Α	369	80.494	57.952	25.770	1.00 24.5	55	C
ATOM	1869	N	ALA	Α	370	76.544	54.478	25.330	1.00 23.0	)2	N
ATOM	1870	CA	ALA	Α	370	75.250	54.031	25.833	1.00 22.9	95	С
ATOM	1871	С	ALA	Α	370	75.427	52.936	26.885	1.00 22.4	19	C
ATOM	1872	0	ALA	A	370	74.777	52.951	27.930	1.00 22.4	15	0
ATOM	1873	СВ	ALA			74.380	53.519	24.674	1.00 21.8	30	C
MOTA	1874	N	LEU			76.311	51.987	26.604	1.00 22.4		N
MOTA	1875	CA	LEU	Α	371	76.561	50.902	27.539	1.00 22.4	16	С
MOTA	1876	С	LEU	A	371	77.268	51.435	28.793	1.00 22.5	8	С
MOTA	1877	0	LEU			76.910	51.071	29.912	1.00 22.7		0
ATOM	1878	СВ	LEU			77.407	49.810	26.863	1.00 22.2		C
MOTA	1879	CG	LEU			76.777	49.111	25.644	1.00 23.0		C
ATOM	1880		LEU			77.821	48.224	24.960	1.00 23.2		C
ATOM	1881		LEU			75.570	48.278	26.074	1.00 22.7		C
ATOM	1882	N	ALA			78.259	52.306	28.607	1.00 22.3		N
ATOM	1883	CA	ALA			79.001	52.863	29.736	1.00 22.6		C
MOTA	1884	C	ALA			78.100	53.669	30.663	1.00 23.0		Ċ
ATOM	1885	0	ALA			78.320	53.705	31.874	1.00 22.8		0
ATOM	1886	CB	ALA			80.140	53.738	29.236	1.00 22.4		C
ATOM	1887	N	MET			77.087	54.316	30.091	1.00 23.3		N
ATOM	1888	CA	MET			76.159	55.113	30.883	1.00 23.3		C
MOTA	1889	C	MET			75.140	54.272	31.654	1.00 23.5		C
ATOM	1890	0	MET			74.361	54.813	32.431	1.00 23.6		0
ATOM	1891	CB	MET				56.127	29.992	1.00 23.6		C
ATOM	1892	CG	MET			75.437	57.212	29.437	1.00 23.2		C
ATOM	1893	SD	MET			76.355	58.296	28.242	1.00 23.2		s
						75.548					
MOTA	1894	CE	MET			76.895	59.426	27.833	1.00 23.1		C
ATOM	1895	N	GLY			75.135	52.956	31.437	1.00 23.7		N
ATOM	1896	CA	GLY			74.210	52.108	32.174	1.00 23.4		C
ATOM	1897	C	GLY			73.258	51.222	31.386	1.00 23.9		C
ATOM	1898	0	GLY			72.709	50.266	31.941	1.00 24.3		0
ATOM .	1899	N	ALA			73034	51.533	30.113	1.00 23.4		N
ATOM	1900	CA	ALA			72.147	50.713	29.296	1.00 24.1		C
ATOM	1901	C .	ALA			72.716		29.212	1.00 24.2		C
ATOM	1902	0	ALA			73.916	49.118	29.022	1.00 24.6		0
MOTA	1903	CB	ALA			72.010		27.898	1.00 22.9		C
MOTA	1904	N	ASP			71.848	48.304	29.369	1.00 24.2		N
ATOM	1905	CA	ASP			72.248	46.905	29.301	1.00 24.3		C
ATOM	1906	C	ASP			72.343	46.495	27.839	1.00 24.2		C
MOTA	1907	0	ASP			73.206	45.708	27.455	1.00 24.2		0
MOTA	1908	CB	ASP			71.227	46.042	30.040	1.00 24.7		C
ATOM	1909	CG	ASP			71.144	46.385	31.518	1.00 25.2		C
ATOM	1910				376` .	71.931	45.821	32.307	1.00 25.9		0
ATOM	1911		ASP			70.304	47.234	31.890	1.00 25.5		0
ATOM	1912	N			377	71.432	47.011	27.025	1.00 24.6		N
ATOM	1913	CA			377	71.472	46.728	25.604	1.00 25.1		C
ATOM	1914	C			377	70.944	47.899	24.795	1.00 25.1		C
ATOM	1915	0			377	70.363	48.838	25.341	1.00 25.1		0
MOTA	1916	CB			377	70.754	45.413	25.240	1.00 24.8		C
MOTA		CG			377	69.354	45.301	25.750	1.00 25.6		C
ATOM	1918		PHE			69.105	44.892	27.056	1.00 25.7		C
MOTA	1919	CD2	PHE	A	377	68.274	45.533	24.901	1.00 25.6	54	C

MOTA	1920	CEl	PHE	Α	377	67.795	44.709	27.512	1.00 25.70		С
ATOM	1921	CE2	PHE	A	377	66.961	45.353	25.346	1.00 25.63		C
MOTA	1922	CZ	PHE	Α	377	66.724	44.939	26.653	1.00 26.08		С
ATOM	1923	N	ILE	Α	378	71.159	47.827	23.488	1.00 25.27		N
ATOM .	1924	CA	ILE	Α	378	70.802	48.895	22.575	1.00 25.00		C-
MOTA	1925	С	ILE	Α	378	69.858	48.454	21.466	1.00 25.29		С
ATOM	1926	0	ILE	Α	378	70.023	47.379	20.895	1.00 25.10		0
ATOM	1927	CB	ILE	А	378	72.099	49.445	21.936	1.00 25.25		С
ATOM	1928	CG1	ILE			73.083	49.820	23.043	1.00 24.86		С
ATOM	1929		ILE			71.802	50.659	21.052	1.00 25.15		C
ATOM	1930		ILE			74.499	49.981	22.560	1.00 26.24		С
MOTA	1931	N	MET			68.859	49.285	21.177	1.00 25.26		N
MOTA	1932	CA	MET			67.922	48.996	20.101	1.00 25.45		C
ATOM	1933	C	MET			68.271	49.957	18.968	1.00 25.68		C
ATOM	1934	Ö	MET			68.464	51.147	19.199	1.00 25.94		0
MOTA	1935	CB	MET			66.467	49.208	20.546	1.00 25.00		Ċ
ATOM	1936 .	CG	MET			65.466	48.982	19.413	1.00 24.97		C
ATOM	1937	SD	MET			63.735	48.885	19.881	1.00 24.78		s
MOTA	1938	CE	MET			63.630	47.182	20.459	1.00 24.70		C
MOTA	1939	N	LEU			68.367	49.443	17.747	1.00 24.04		N
ATOM	1940	CA	LEU			68.712	50.287	16.606	1.00 26.36		C
MOTA	1941	C	LEU			67.836	49.997	15.398	1.00 26.33		C
MOTA	1942	0	LEU				48.852	15.160	1.00 25.51		0
ATOM	1943	CB	LEU			67.452 70.183	50.090	16.208	1.00 25.51		C
	1943		LEU				50.090	17.268			C
MOTA		CG				71.270			1.00 27.60		
MOTA	1945		LEU			71.391	49.039	18.110	1.00 28.42		C
ATOM	1946		LEU			72.609	50.595	16.608	1.00 27.51		C
MOTA	1947	N	GLY			67.529	51.048	14.644	1.00 26.78		N
MOTA	1948	CA			381	66.720	50.907	13.446	1.00 27.90		C
ATOM	1949	C			381	67.566	51.146	12.206	1.00 28.83		C
ATOM	1950	0	GLY			67.879	50.215	11.465	1.00 28.61		0
ATOM	1951	N	ARG			67.950	52.399	11.991	1.00 30.04		N
ATOM	1952	CA	ARG			68.766	52.775	10.837	1.00 31.91		C
ATOM	1953	C	ARG			69.988	51.873	10.639	1.00 31.42		C
ATOM	1954	0	ARG			70.278	51.442	9.522	1.00 31.49		0
MOTA	1955	CB	ARG			69.220	54.232	10.971	1.00 34.20		C
ATOM	1956	CG	ARG			70.290	54.630	9.964	1.00 38.29		C
MOTA	1957	CD	ARG			70.947	55.962	10.312	1.00 41.29		C
MOTA	1958	NE	ARG			72.287	56.062	9.729	1.00 44.45		N
ATOM	1959	CZ	ARG			72.542	56.128	8.423	1.00 45.83		C
MOTA	1960		ARG			71.545	56.111	7.544	1.00 46.63		N
MOTA	1961		ARG			73.796	56.202	7.994	1.00 46.53		N
ATOM	1962	N			383	70.700	51.596	11.727	1.00 30.70		N
MOTA	1963	CA			383	71.892	50.753	11.692	1.00 29.42	•	C
MOTA	1964	C			383	71.652	49.421	10.978	1.00 29.27		C
MOTA	1965	0			383	72.448	49.013	10.128	1.00 29.04		0
ATOM	1966	CB			383	72.380	50.487	13.124	1.00 28.61		C
MOTA	1967	CG			383	73.607	49.602	13.223	1.00 27.85		С
MOTA	1968		TYR			74.894	50.134	13.107	1.00 27.60		С
ATOM	1969		TYR			73.479	48.228	13.419	1.00 27.75		С
ATOM	1970		TYR			76.020	49.317	13.185	1.00 27.67		C
MOTA	1971		TYR			74.592	47.403	13.495	1.00 27.39		С
ATOM	1972	CZ	TYR	A	383	75.859	47.948	13.377	1.00 27.90		C
MOTA	1973	OH	TYR	A	383	76.958	47.118	13.438	1.00 27.45		0
MOTA	1974	N	PHE	A	384	70.560	48.747	11.327	1.00 28.44		N
ATOM	1975	CA	PHE	A	384	70.232	47.454	10.733	1.00 28.47		С
ATOM	1976	C	PHE	A	384 -	69.521	47.555	9.381	1.00 28.91		C

MOTA	1977	0	PHE	A	384		69.627	46.650	8.555	1.00	28.72			0
MOTA	1978	CB	PHE	Α	384		69.375	46.636	11.705	1.00	27.39			С
MOTA	1979	CG	PHE	Α	384		70.132	46.130	12.906	1.00	26.72			С
MOTA	1980	CD1	PHE	А	384		71.098	45.132	12.768	1.00	25.87			C
ATOM	1981	CD2	PHE	A	384		69.886	46.656	14.173	1.00	25.64			C
ATOM	1982		PHE				71.807	44.664	13.868	1.00	25.34			C
MOTA	1983	CE2	PHE				70.591	46.193	15.285	1.00	25.24			C
ATOM	1984	CZ	PHE				71.554	45.195	15.134	1.00	24.96			C
ATOM	1985	N	ALA				68.804	48.653	9.158		29.46			N
ATOM	1986 .	CA	ALA				68.081	48.852	7.905		30.43			C
ATOM	1987	C	ALA				69.024	48.849	6.701		31.20			Ċ
ATOM	1988	0	ALA				68.626	48.506	5.592		31.54			ō
ATOM	1989	СВ	ALA				67.299	50.166	7.958		29.86			C
MOTA	1990	N	ARG				70.278	49.226	6.934		32.25	·		N
ATOM	1991	CA	ARG				71.291	49.281	5.883		32:76			C
ATOM	1991	CA	ARG				71.725	47.907	5.381		33.11			C
											32.93			0
ATOM	1993	0	ARG			-	72.310	47.794	4.305		33.15			C
ATOM	1994	CB			386		72.542	49.995	6.392					
ATOM	1995	CG	ARG				72.363	51.434	6.832		34.37			C
MOTA	1996	CD	ARG				73.645	51.881	7.510		34.93			C
MOTA	1997	NE	ARG				74.002		8.567		36.03			N
MOTA	1998	CZ	ARG				75.245	50.652	8.938		36.05			С
MOTA	1999		ARG				76.278	51.233	8.338		35.62			N
MOTA	2000		ARG				75.451	49.774	9.910		35.65			N
ATOM	2001	N			387		71.447	46.867	6.158		33.64			N
MOTA	2002	CA			387		71.875	45.525	5.787		34.50			С
MOTA	2003	C			387		71.012	44.785	4.768		35.58			С
MOTA	2004	0			387		69.818	45.037	4.623		35.41			0
MOTA	2005	CB	PHE	A	387		72.040	44.665	7.046		33.89			С
MOTA	2006	CG	PHE	A	387		72.940	45.276	8.091	1.00	33.56		•	C
ATOM	2007	CD1	PHE	Α	387		74.033	46.058	7.722	1.00	33.59			С
ATOM	2008	CD2	PHE	Α	387		72.707	45.050	9.444	1.00	33.20			C
MOTA	2009	CE1	PHE	Α	387		74.881	46.607	8.689	1.00	33.28			C
MOTA	2010	CE2	PHE	A	387`		73.547	45.592	10.417	1.00	32.86			C
MOTA	2011	CZ	PHE	Α	387		74.636	46.372	10.040	1.00	33.10			C
MOTA	2012	N	GLU	Α	388		71.647	43.859	4.064	1.00	37.23			N
ATOM	2013	CA	GLU	Α	388		70.979	43.061	3.048	1.00	38.92			C
ATOM	2014	C	GLU	Α	388		69.769	42.341	3.632	1.00	38.75			C
MOTA	2015	0	GLU	Α	388	•	68.737	42.209	2.972	1.00	38.22			0
ATOM	2016	CB	GLU	Α	388		71.957	42.034	2.473	1.00	40.97			C
MOTA	2017	CG	GLU	Α	388		71.424	41.264	1.272	1.00	44.75			C
MOTA	2018	CD	GLU	A	388		72.279	40.056	0.934		47.13			C
MOTA	2019	OE1	GLU				72.425	39.172	1.808		48.77			0
ATOM	2020		GLU				72.803	39.985	-0.202		48.96			0
ATOM	2021	N			389		69.899	41.886	4.876		38.62			N
MOTA	2022	CA			389		68.823	41.159	5.534		38.62			C
ATOM	2023	C			389		67.615	41.987	5.964		38.96			C
ATOM	2024	ō			389		66.621	41.424	6.413		39.16			0
MOTA	2025	CB			389		69.369	40.375	6.732		37.80			C,
ATOM	2026	CG			389		70.398	39.320	6.347		36.96			C
ATOM	2027	CD			389		71.834		6.504		36.79			C
ATOM	2027		GLU				72.100	41.004	6.310		36.41			0
MOTA	2028		GLU				72.704	38.958	6.808		35.78			0
ATOM	2029	N N			390		67.679	43.310	5.843		39.56			N
											40.72			C
MOTA	2031	CA C			390		66.515	44.105 43.815	6.216		40.72			C
MOTA	2032				390		65.467		5.138					
ATOM	2033	0	SER	A	390		65.807	43.599	3.973	1.00	41.48			0

MOTA	2034	CB	SER	A	390	66.844	45.598	6.278	1.00 40.08	C
MOTA	2035	OG	SER	A	390	67.105	46.130	5.000	1.00 40.77	0
MOTA	2036	N	PRO	A	391	64.181	43.804	5.515	1.00 42.67	N
ATOM	2037	CA	PRO	A	391	63.073	43.523	4.595	1.00 43.86	С
ATOM	2038	С	PRO			62.716	44.593	3.567	1.00 44.88	C
ATOM	2039	0	PRO			61.651	44.530	2.959	1.00 45.36	0
ATOM	2040	СВ	PRO			61.917	43.245	5.550	1.00 43.53	C
ATOM	2041	CG	PRO			62.172	44.253	6.634	1.00 42.86	Ċ
						63.672	44.149	6.858	1.00 42.43	C
ATOM ·	2042	CD			391			3.361		N
ATOM	2043	N	THR			63.588	45.570		1.00 46.16	
ATOM	2044	CA			392	63.280	46.619	2.402	1.00 47.44	C
MOTA	2045	C			392	63.962	46.419	1.057	1.00 48.73	С
MOTA	2046	0	THR	A	392	64.940	45.680	0.939	1.00 48.53	0
ATOM	2047	CB	THR	А	392	63.646	48.010	2.955	1.00 47.37	С
MOTA	2048	OG1	THR	Α	392	65.056	48.081	3.190	1.00 47.28	0
ATOM	2049	CG2	THR	Α	392	62.901	48.266	4.264	1.00 47.46	С
ATOM	2050	N.	ARG	Α	393	63.430	47.085	0.041	1.00 50.37	N
ATOM	2051	CA	ARG	А	393	63.966	46.980	-1.305	1.00 52.41	С
ATOM	2052	C			393	65.285	47.716	-1.481	1.00 52.98	C
ATOM	2053		ARG			65.459	48.846	-1.020	1.00 52.98	0
ATOM	2054	CB			393	62.936	47.494	-2.318	1.00 53.44	C
ATOM	2055	CG	ARG			61.734	46.567	-2.475	1.00 54.94	C
									1.00 56.14	C
ATOM	2056	CD	ARG			60.591	47.199	-3.269		
MOTA	2057	NE			393	61.022	47.742	-4.554	1.00 57.05	N
ATOM	2058	CZ	ARG			61.422	48.997	-4.739	1.00 57.73	С
MOTA	2059		ARG			61.444	49.848	-3.720	1.00 58.03	N
MOTA	2060	NH2	ARG	Α	393	61.803	49.402	-5.943	1.00 58.01	N
MOTA	2061	N	LYS	Α	394	66.220	47.046	-2.141	1.00 53.68	N
MOTA	2062	CA	LYS	Α	394	67.526	47.616	-2.417	1.00 54.28	C
MOTA	2063	C	LYS	Α	394	67.338	48.454	-3.674	1.00 54.83	C
MOTA	2064	0	LYS	Α	394	66.910	47.943	-4.704	1.00 54.68	0
ATOM	2065	CB			394	68.532	46.495	-2.670	1.00 53.95	C
ATOM	2066	CG			394	69.979	46.924	-2.607	1.00 53.65	С
ATOM	2067	CD			394	70.900	45.769	-2.961	1.00 53.38	C
ATOM	2068	CE			394	70.731	44.601	-2.009	1.00 52.92	C
ATOM	2069	NZ			394	71.581	43.452	-2.415	1.00 52.52	N
					395	67.640	49.742		1.00 55.84	N
MOTA	2070	N						-3.585		
MOTA	2071	CA			395	67.471	50.629	-4.724	1.00 57.03	C
MOTA	2072	С			395	68.749	51.379	-5.052	1.00 57.77	C
ATOM	2073	Ο,			395	69.439	51.859	-4.159	1.00 58.06	0
MOTA	2074	CB			395	66.352	51.653	-4.457	1.00 57.18	C.
MOTA	2075		VAL			66.227	52.612	-5.632	1.00 57.63	C
MOTA	2076	CG2	VAL	А	395	65.036	50.926	-4.220	1.00 57.44	 С
MOTA	2077	N	THR	Α	396	69.055	51.480	-6.340	1.00 58.78	N
MOTA	2078	CA	THR	Α	396	70.255	52.176	-6.786	1.00 59.74	С
ATOM	2079	С	THR	A	396	69.940	53.611	-7.189	1.00 60.37	С
MOTA	2080	0			396	69.146	53.851	-8.096	1.00 60.74	0
ATOM	2081	CB			396	70.900	51.466	-7.989	1.00 59.62	С
ATOM	2082	OG1			396	71.197	50.110	-7.639	1.00 59.68	0
ATOM	2083	CG2			396	72.184	52.173	-8.394	1.00 59.73	C
ATOM	2083	N			397	70.565	54.559	-6.502	1.00 61.02	N
									1.00 61.02	C
ATOM	2085	CA			397	70.366	55.974	-6.783		
MOTA	2086	C			397	71.659	56.562	-7.342	1.00 61.67	C
ATOM	2087	0			397	72.589	56.872	-6.595	1.00 61.90	0
ATOM	2088	CB			397	69.962	56.744	-5.506	1.00 61.92	C
MOTA	2089		ILE			68.655	56.173	-4.950	1.00 62.18	C
MOTA	2090	CG2	ILE	A	397	69.792	58.223	-5.817	1.00 62.12	С

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ATOM	2091	CD1	ILE	Α	397	68.171	56.858	-3.689	1.00	62.37			С
ATOM	2092	N	ASN	Α	398	71.700	56.708	-8.663	1.00	61.56			N
ATOM	2093	CA	ASN	Α	398	72.856	57.247	-9.375	1.00	61.04			C
ATOM	2094	С	ASN	Α	398	74.211	56.789	-8.831	1.00	60.11			С
ATOM	2095	0	ASN	Α	398	74.960	57.570	-8.239	1.00	60.00			0
ATOM	2096	CB	ASN			72.795	58.784	-9.415	1.00	62.12			С
MOTA	2097	CĢ	ASN			72.965	59.425	-8.047	1.00	62.95			С
ATOM	2098	•	ASN			72.154	59.222	-7.145		63.58			0
ATOM	2099	ND2				74.026	60.216	-7.892		63.27			N
ATOM	2100	N	GLY			74.516	55.512	-9.039		58.84			N
ATOM	2101	CA	GLY			75.786	54.965	-8.593		57.27			C
ATOM	2102	C	GLY			75.861	54.494	-7.153		56.12			C
ATOM	2103	0	GLY			76.847	53.867	-6.761	-	56.17			0
ATOM	2104		SER			74.835	54.788	-6.359		54.73			
ATOM	2104	CA	SER			74.833	54.788						N
ATOM	2105	C	SER					-4.957		52.89			C
						73.686	53.444	-4.603		51.55			C
ATOM	2107	0	SER			72.517	53.775	-4.785		51.45			0
MOTA	2108	CB			400	74.779	55.608	-4.047		52.78			C
ATOM	2109	OG	SER			75.979	56.353	-4.134		52.96	•		0
MOTA	2110	N	VAL			74.030	52.268	-4.094		50.01			N
MOTA	2111	CA			401	73.025	51.298	-3.697		48.59			C
MOTA	2112	C	VAL			72.507	51.704	-2.320		48.17			С
MOTA	2113	0	VAL			73.275	51.816	-1.360		47.91			0
ATOM	2114	CB	VAL			73.620	49.883	-3.637	1.00	48.31			C
MOTA	2115		·VAL			72.563	48.892	-3.182	1.00	47.71			С
MOTA	2116	CG2	VAL			74.167	49.499	-5.007	1.00	47.95			С
MOTA	2117	N	MET	Α	402	71.202	51.941	-2.238	1.00	47.38			N
MOTA	2118	CA	MET	Α	402	70.566	52.360	-0.998	1.00	46.51			С
MOTA	2119	C	MET	А	402	69.492	51.365	-0.589	1.00	45.72			С
MOTA	2120	Ó	MET	Α	402	69.161	50.440	-1.333	1.00	45.52			0
MOTA	2121`	CB	MET	Α	402	69.893	53.724	-1.179	1.00	47.39			С
MOTA	2122	CG	MET	Α	402	70.722	54.785	-1.882	1.00	47.80			С
MOTA	2123	SD	MET	А	402	72.046	55.436	-0.875	1.00	49.53			S
MOTA	2124	CE	MET			71.130	56.502	0.246		48.12			C
ATOM	2125	N	LYS			68.953	51.568	0.606		44.48			N
ATOM	2126	CA	LYS			67.879	50.735	1.118		43.18			C
MOTA	2127	С	LYS			66.843	51.671	1.713		42.91			C
ATOM	2128	ō	LYS			67.178	52.736	2.232		42.51			0
ATOM	2129	CB	LYS			68.387	49.759	2.180		42.62	•		C
ATOM	2130	CG	LYS			69.316	48.691	1.632		41.97			C
ATOM	2131	CD	LYS			69.087	47.352	2.306		41.27			C
MOTA	2132	CE	LYS			67.729						-	C
ATOM	2132	NZ					46.777	1.941		40.54			
			LYS GLU			67.534	45.407	2.492		39.50			N
ATOM	2134	N				65.580	51.280	1.622		42.89			N
ATOM	2135	CA	GLU			64.500	52.097	2.146		42.99			C
MOTA	2136	C	GLU			64.451	52.019	3.661	•	42.20			C
MOTA	2137	0	GLU			64.760	50.987	4.254		41.68			0
MOTA	2138	CB	GLU			63,166	51.623	1.580		44.40			C
MOTA	2139	CG	GLU			63.131	51.559	0.071		46.68			С
ATOM	2140	CD	GLU			61.810	51.042	-0.446		48.00			C
MOTA	2141		GLU			61.485	49.856	-0.191		49.02			0
MOTA	2142	OE2	GLU			61.095	51.827	-1.101		49.09			0
MOTA	2143	N	TYR			64.061	53.124	4.284		41.51			N
MOTA	2144	CA	TYR	A	405	63.949	53.180	5.729	1.00	40.50			С
MOTA	2145	C	TYR			62.918	54.221	6.123	1.00	40.07			С
MOTA	2146	0	TYR	А	405	63.100	55.416	5.882	1.00	40.71			0
ATOM	2147	CB	TYR	А	405	65.294	53.524	6.365	1.00	40.22			С

ATOM	2148	CG	TYR	A	405		65.231	53.579	7.872	1.00 40.08		С
MOTA	2149	CD1	TYR	Α	405		64.847	52.463	8.611	1.00 39.84		C
MOTA	2150	CD2	TYR	Α	405		65.539	54.750	8.561	1.00 40.31	,	C
MOTA	2151	CE1	TYR	Α	405		64.771	52.508	9.998	1.00 39.70		C
MOTA	2152	CE2	TYR	A	405		65.466	54.807	9.949	1.00 40.16		C
MOTA	2153	CZ	TYR	Α	405		65.080	53.681	10.659	1.00 39.81		C
MOTA	2154	OH	TYR	Α	405		64.990	53.734	12.027	1.00 39.77		0
MOTA	2155	N	TRP	Α	406		61.830	53.764	6.729	1.00 38.92		N
MOTA	2156	CA	TRP	Α	406		60.773	54.666	7.153	1.00 38.11		C
MOTA	2157	C	TRP	Α	406		60.373	54.354	8.588	1.00 38.26		C
ATOM	2158	0	TRP	A	406		60.439	53.202	9.026	1.00 37.61		0
MOTA	2159	CB	TRP	Α	406		59.565	54.545	6.212	1.00 36.65		C
ATOM	2160	CG	TRP	Α	406		58.932	53.186	6.184	1.00 35.15		C
ATOM	2161	CD1	TRP	Α	406		57.972	52.715	7.028	1.00 34.75		C
MOTA	2162	CD2	TRP	Α	406		59.246	52.111	5.293	1.00 34.82		C
ATOM	2163	NE1	TRP	Α	406		57.667	51.414	6.722	1.00 34.33		N
MOTA	2164	CE2	TRP	Α	406		58.437	51.015	5.661	1.00 34.71		C
MOTA	2165	CE3	TRP	Α	406		60.135	51.965	4.218	1.00 34.73		C
ATOM	2166	CZ2	TRP	А	406		58.488	49.784	4.994	1.00 34.60		C
MOTA	2167	CZ3	TRP	А	406		60.186	50.740	3.551	1.00 34.68		C
MOTA	2168	CH2	TRP	Α	406		59.366	49.666	3.946	1.00 34.70		С
MOTA	2169	N	GLY	A	407		59.978	55.392	9.316	1.00 38.58		N
MOTA	2170	CA	GLY	А	407		59.571	55.221	10.695	1.00 39.46		C
MOTA	2171	C	$\mathtt{GLY}$	A	407	٠.	58.182	54.625	10.820	1.00 40.35		C
ATOM	2172	0	GLY	A	407		57.402	54.627	9.867	1.00 40.02		0
ATOM	2173	N	GLU	A	408.		57.878	54.102	12.003	1.00 41.35		Ŋ
MOTA	2174	CA	GLU	А	408		56.578	53.506	12.271	1.00 42.48		, C
MOTA	2175	С	GLU	Α	408		55.513	54.585	12.394	1.00 43.53		C
MOTA	2176	0	GLU	A	408		54.320	54.302	12.334	1.00 43.54		0
ATOM	2177	CB	GLU	A	408		56.641	52.682	13.555	1.00 42.13		C
MOTA	2178	CG	GLU	Α	408	•	57.446	51.408	13.410	1.00 41.70		C
ATOM	2179	CD	GLU	A	408		56.789	50.416	12.464	1.00 41.39		C
ATOM	2180	OE1	GLU	Α	408		55.688	49.927	12.785	1.00 41.50		0
ATOM	2181	QE2	GLU	Α	408		57.370	50.126	11.401	1.00 40.96		. 0
ATOM	2182	N	GLY	Α	409		55.954	55.827	12.562	1.00 45.08		N
MOTA	2183	CA	GLY	Α	409		55.022	56.932	12.681	1.00 47.32		C
MOTA	2184	C	GLY	Α	409		54.711	57.588	11.345	1.00 48.91		C
MOTA	2185	0			409		53.891	58.502	11.274	1.00 48.67		0
MOTA	2186	N	SER	A	410		55.365	57.130	10.281	1.00 50.68		N
MOTA	2187	CA	SER	A	410		55.132	57.699	8.958	1.00 52.76		C
MOTA	2188	C			410		53.849		8.373	1.00 54.23		C
MOTA	2189	0			410		53.454		8.689	1.00 53.75		0
MOTA	2190	CB			410		56.301		8.015	1.00 52.65		C
MOTA	2191	OG			410		56.325	56.026	7.646	1.00 53.09		0
MOTA	2192	N			411		53.200		7.520	1.00 56.27		И
MOTA	2193	CA			411		51.960		6.889	1.00 58.56		C
MOTA	2194	C			411		52.188		6.088	1.00 60.08		C
MOTA	2195	0			411		51.270		5.916	1.00 60.54		0
MOTA	2196	CB			411		51.430		5.973	1.00 58.70		C
MOTA	2197	OG			411		52.376		4.974	1.00 59.09		O
MOTA	2198	N			412		53.418		5.612	1.00 61.61		N
MOTA	2199	CA			412		53.770		4.831	1.00 63.31		C
MOTA	2200	C			412		53.527		5.609	1.00 64.68		
MOTA	2201	0			412		53.565		5.043	1.00 64.66		C
MOTA	2202	CB			412		55.236		4.385	1.00 62.76		C
MOTA	2203	CG			412		55.694		3.581	1.00 62.41		C
MOTA	2204	CD	ARG	Α	412		57.020	53.948	2.877	1.00 61.98		

ATOM	2205	NE	ARG	Α	412	57.408	52.776	2.097	1.00	61.77		N
ATOM	2206	CZ	ARG	Α	412	58.493	52.701	1.332	1.00	62.01		С
ATOM	2207	NH1	ARG	A	412	59.321	53.736	1.229	1.00	61.70		N
ATOM	2208		ARG			58.751	51.581	0.669	1.00	62.05		N
ATOM	2209	N	ALA	Α	413	53.273	53.681	6.908		66.59		N
ATOM	2210	CA			413	53.016	52.532	7.770		68.37		C
ATOM	2211	C			413	51.774	52.795	8.617		69.80		C
ATOM	2212	0			413	50.907	53.587	8.232		70.13		0
ATOM	2213	CB			413	54.222	52.279	8.672		68.21		C
ATOM	2214	N			414	51.697	52.124	9.767		71.35		N
ATOM	2215	CA .				50.586	52.267	10.715		72.93		С
ATOM	2216	C			414	49.190	52.288	10.097		73.77		С
MOTA	2217	0			414	48.213	52.609	10.774		73.88		0
MOTA	2218	CB	ARG	Α	414	50.783	53.530	11.570	1.00	73.43		С
MOTA	2219	CG	ARG			51.031	54.815	10.779	1.00	74.17		C
MOTA	2220	CD	ARG	Α	414	51.446	55.967	11.688	1.00	74.85		С
ATOM	2221	NE	ARG	Α	414	50.307	56.638	12.308	1.00	75.54		N
MOTA	2222	CZ	ARG	Α	414	49.508	57.492	11.675	1.00	75.93		C
MOTA	2223	NHl	ARG	Α	414	49.724	57.784	10.398	1.00	76.05		N
MOTA		NH2				48.495	58.059	12.319		76.11		N
MOTA	2225	N			415	49.098	51.936	8.819		74.50		N
ATOM	2226	CA			415	47.818	51.923	8.124		75.19		C
ATOM	2227	C			415	47.577	50.540	7.515		75.37		C
ATOM	2228	0			415	47.344						
			ASN		•		50.406	6.311		75.45		0
MOTA	2229	CB				47.809	52.996	7.028		75.72		C
ATOM	2230	CG	ASN			46.402	53.424	6.634		76.17		C
MOTA	2231		ASN			46.214	54.171	5.671		76.40		0
ATOM	2232		ASN			45.406	52,958	7 _, .385		76.16		N
MOTA	2233	N			416	47.644	49.516	8.361		75.41		N
MOTA	2234	CA			416	47.437	48.136	7.931	1.00	75.40		С
ATOM	2235	C	TRP	Α	416	46.062	47.625	8.366	1.00	75.38		C
MOTA	2236	0	TRP	Α	416	45.571	47.959	9.448	1.00	75.34		0
MOTA	2237	CB	TRP	A	416	48.532	47.232	8.515	1.00	75.24		C
ATOM	2238	CG	TRP	Α	416	48.733	47.426	9.990	1.00	74.99		С
MOTA	2239	CD1	TRP	Α	416	49.406	48.449	10.599	1.00	74.96		С
ATOM	2240	CD2	TRP			48.190	46.620	11.044		74.76		С
ATOM	2241		TRP			49.311	48.333	11.966		74.83		N
ATOM	2242	CE2	TRP			48.570	47.220	12.267		74.77		C
ATOM	2243	CE3	TRP			47.415	45.453	11.075		74.57		C
ATOM	2244		TRP			48.200	46.691	13.510		74.66		C
ATOM	2245		TRP			47.047	44.927	12.313				
MOTA	2245	CH2					45.549			74.66		C
ATOM						47.442		13.513		74.65		C
	2247	N	GLU			54.518	61.394	12.341		65.44		N
ATOM	2248	CA	GLU-			55.528	61.368	13.394		65.56	•	C
ATOM	2249	C	GLU			56.862	60.844	12.879		64.74		C
ATOM	2250	0			431	57.864	60.865	13.595		64.65		0
ATOM	2251	CB	GLU			55.072	60.484	14.557		66.48		С
ATOM	2252	CG	GLU			53.806	60.944	15.256	1.00	68.09		С
MOTA	2253	CD	GLU			53.483	60.087	16.469	1.00	69.15		С
ATOM	2254	OE1	GLU	А	431	53.319	58.854	16.306	1.00	69.66		0
MOTA	2255	OE2	GLU	А	431	53.397	60.647	17.586	1.00	69.60		0
MOTA	2256	N	$\operatorname{GLY}$	Α	432	56.873	60.368	11.641	1.00	63.84		N
MOTA	2257	CA	$\operatorname{GLY}$	Α	432	58.100	59.842	11.080		62.59		С
MOTA	2258	C	GLY			58.315	60.225	9.633		61.80		С
MOTA	2259	0	GLY			57.421	60.765	8.977		61.75		0
MOTA	2260	N	VAL			59.513	59.938	9.135		60.79		N
ATOM	2261	CA	VAL			59.867	60.246	7.758		59.34		C
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MOTA	2262	C	VAL	А	433	60.128	58.968	6.964	1.00	58.28		С
MOTA	2263	0	VAL	A	433	60.193	57.874	7.527	1.00	58.02		0
MOTA	2264	CB	VAL	A	433	61.124	61.149	7.700	1.00	59.34		C
MOTA	2265	CG1	VAL	Α	433	60.851	62.462	8.413	1.00	59.24		С
ATOM	2266	CG2	VAL	Α	433	62.309	60.442	8.336	1.00	59.25		C
ATOM	2267	N.	ASP	Α	434	60.263	59.122	5.651	1.00	56.94		N
ATOM	2268	CA	ASP	Α	434	60.528	58.010	4.747	1.00	55.49		С
ATOM	2269	С	ASP			61.778	58.380	3.957		54.43		, C
ATOM	2270	0	ASP			61.777	59.359	3.210		54.60		0
ATOM	2271	СВ	ASP			59.333	57.808	3.809		55.70		C
ATOM	2272	CG	ASP			59.529	56.653	2.849		55.96		C
ATOM	2273		ASP			59.987	55.578	3.288		56.51		0
ATOM	2274		ASP			59.212	56.812	1.652		56.42		ō
ATOM	2275	N			435	62.845	57.602	4.119		52.71		N
ATOM	2276	CA			435	64.099	57.908	3.440		50.99	•	C
ATOM	2277	C			435	64.910	56.705	2.962		49.63		C
ATOM	2278	0			435		55.581	2.891		48.99		0
MOTA	2279	CB			435	64.971	58.757	4.366		51.10		C
										50.72		0
ATOM	2280	OG			435	65.160	58.097	5.608		48.33		
ATOM	2281	N			436 .	66.172	56.970	2.640				N
ATOM	2282	CA .			436	67.091	55.947			47.20		C
MOTA	2283	C			436	68.375	55.936	2.984		45.70		С
ATOM	2284	0			436	68.863	56.987	3.400		45.68		0
ATOM	2285	CB			436	67.452	56.211	0.699		48.21		C
MOTA	2286	CG			436	66.289	56.130	-0.260		49.01		C
MOTA	2287	CD1	TYR			65.771	54.895	-0.656		49.13		C
MOTA	2288	CD2	TYR			65.701	57.288	-0.769		49.35		C
MOTA	2289	CE1				64.694	54.816	-1.538		49.77		C
MOTA	2290	CE2	TYR	А	436	64.622	57.221	-1.650		49.98		C
MOTA	2291	CZ	TYR	Α	4:36	64.125	55.982	-2.029		49.99		C
MOTA	2292	OH	TYR	Α	436	63.054	55.911	-2.891	1.00	50.64		0
MOTA	2293	N	VAL	Α	437	68.913	54.743	3.214	1.00	43.68		N
MOTA	2294	CA	VAL	Α	437	70.164	54.591	3.944	1.00	41.96		С
MOTA	2295	C	VAL	A	437	71.139	53.869	3.025	1.00	40.88		C
ATOM	2296	0	VAL	Α	437	70.741	53.013	2.238	1.00	40.43		0
MOTA	2297	CB	VAL	Α	437	69.992	53.765	5.245	1.00	41.57		C
MOTA	2298	CG1	VAL	Α	437	69.165	54.547	6.252	1.00	41.59		C
MOTA	2299	CG2	VAL	Α	437	69.341	52.433	4.936	1.00	41.15		C
MOTA	2300	N	PRO	Α	438	72.431	54.210	3.107	1.00	40.34		· N
ATOM	2301	CA	PRO	Α	438	73.428	53.559	2.252	1.00	39.68		C
ATOM	2302	С	PRO	A	438	73.553	52.068	2.546	1.00	39.03		C
MOTA	2303	0			438	73.591	51.656	3.708	1.00	38.81		0
ATOM	2304	CB			438	74.706	54.329	2.570	1.00	39.92		С
ATOM	2305	CG			438	74.512	54.693	4.014	1.00	40.33		С
MOTA	2306	CD			438	73.072	55.149			40.10		C
ATOM	2307	N			439	73.606	51.267	1.486		38.09		N
ATOM	2308	CA			439	73.736	49.821	1.614		37.58		C
MOTA	2309	C			439	75.059	49.499	2.299		37.43		C
ATOM	2310	0			439	76.098	50.048	1.948		37.52		0
ATOM	2311	CB			439	73.688	49.170	0.229		36.98		Ċ
MOTA	2312	CG			439	73.817	47.666	0.237		36.27		C
ATOM	2312	CD1			439	72.869	46.871	0.870		36.31		C
ATOM	2313		TYR			74:879	47.034	-0.414		36.64		C
ATOM	2314		TYR			74.879	45.479	0.856		36.58		C
								-0.434		36.33		C
MOTA	2316	CE2			439	74.989	45.646					C
ATOM	2317	CZ			439	74.030	44.877	0.202		36.46		0
MOTA	2318	OH	TIK	A	439	74.134	43.506	0.187	1.00	37.16		J

ATOM	2319	N	ALA	A	440	75.024	48.598	3.272	1.00 37.4	6		N
MOTA	2320	CA	ALA	Α	440	76.236	48.251	4.002	1.00 37.4	2		С
MOTA	2321	С	ALA	A	440	76.672	46.809	3.794	1.00 37.2	0		С
MOTA	2322	0	ALA	Α	440	77.760	46.424	4.213	1.00 37.1	5		0
MOTA	2323	CB	ALA	A	440	76.033	48.523	5.494	1.00 37.1	8		C
ATOM	2324	N	GLY	А	441	75.828	46.016	3.145	1.00 37.0	4		N
MOTA	2325	CA	GLY			76.169	44.624	2.926	1.00 37.0			С
ATOM	2326	C	GLY	A	441	75.475	43.746	3.950	1.00 37.2			С
MOTA	2327	Ο.	GLY			74.415		4.456	1.00 37.1			0
MOTA	2328	N	LYS			76.067	42.598	4.265	1.00 37.5			N
ATOM	2329	CA	LYS			75.469	41.687	5.232	1.00 37.8			С
ATOM	2330	C	LYS			75.707	42.113	6.677	1.00 37.1			С
ATOM	2331	0	LYS			76.746	42.683	7.013	1.00 36.6			0
ATOM	2332	CB	LYS			75.995	40.266	5.017	1.00 39.1			C
ATOM	2333	CG	LYS			75.839	39.789	3.584	1.00 41.5			C
ATOM	2334	CD	LYS			75.692	38.280	3.495	1.00 43.2			С
ATOM	2335	CE	LYS			74.316	37.842	3.976	1.00 44.4			C
MOTA	2336	NZ	LYS			74.126	36.365	3.858	1.00 45.9			N
MOTA	2337	N	LEU			74.724	41.823	7.524	1.00 36.3			N
ATOM	2338	CA	LEU			74.774	42.161	8.940	1.00 35.7			C
MOTA	2339	C	LEU			76.055	41.701	9.645	1.00 35.7			С
MOTA	2340	0	LEU			76.723	42.493	10.314	1.00 35.0			0
ATOM	2341	CB	LEU			73.545	41.571	9.640	1.00 34.5		•	С
MOTA	2342	CG	LEU			73.386	41.723	11.157	1.00 34.0			С
MOTA	2343	CD1	LEU		-	71.921	41.572	11.526	1.00 33.3			С
MOTA	2344	CD2	TEU	Α	443	74.234	40.685	11.883	1.00 33.4			С
MOTA	2345 ,	N	LYS			76.396	40.428	9.479	1.00 35.8			N
MOTA	2346	CA	LYS			77.572	39.840	10.116	1.00 36.5			С
MOTA	2347	C	LYS	Α	444	78.837	40.702	10.158	1.00 36.3			С
MOTA	2348	0	LYS	Α	444	79.285	41.100	11.232	1.00 36.2	7 ,		0
MOTA	2349	CB	LYS	Α	444	77.910	38.500	9.455	1.00 37.6	2		С
MOTA	2350	CG	LYS	Α	444	78.998	37.715	10.180	1.00 39.3	4		С
ATOM	2351	CD	LYS	A	444	79.322	36.415	9.452	1.00 40.9	7		С
MOTA	2352	CE	LYS	Α	444	80.227	35.523	10.285	1.00 41.6	4		C
MOTA	2353	NZ	LYS	Α	444	81.483	36.221	10.689	1.00 42.4			N
MOTA	2354	N	ASP	Α	445	79.406	40.985	8.991	1.00 35.8	0		И
ATOM	2355	CA	ASP	Α	445	80.638	41.762	8.892	1.00 35.7	2		C
MOTA	2356	C	ASP	À	445	80.567	43.135	9.546	1.00 34.6	0		С
MOTA	2357	0			445	81.541	43.593	10.148	1.00 34.0			0
ATOM	2358	CB	ASP	A	445	81.033	41.918	7.421	1.00 37.6	1 .		С
MOTA	2359	CG	ASP	Α	445	81.167	40.580	6.711	1.00 39.4			C
MOTA	2360		ASP			82.084	39.804	7.066	1.00 39.7			0
MOTA	2361	OD2	ASP			80.343	40.301	5.810	1.00 40.6	8		0
ATOM	2362	N			446	79.420	43.792	9.415	1.00 33.1			N
MOTA	2363	CA	ASN	A	446	79.231	45.117	9.991	1.00 32.2			С
ATOM	2364	C	ASN	Α	446	79.121	45.054	11.508	1.00 31.8	5		С
MOTA	2365	0			446	79.757	45.833	12.217	1.00 31.3			0
ATOM	2366	CB			446	77.983	45.759	9.398	1.00 32.1			С
ATOM	2367	CG			446	78.181	46.173	7.956	1.00 32.2			С
ATOM	2368		ASN			78.690	47.264	7.678	1.00 32.3			0
MOTA	2369	ND2	ASN			77.797	45.300	7.029	1.00 30.9			N
ATOM	2370	N			447	78.318	44.120	12.004	1.00 31.2			N
MOTA	2371	CA			447	78.151	43.965	13.436	1.00 31.2			С
ATOM	2372	C			447	79.477	43.588	14.104	1.00 31.6			С
ATOM	2373	0			447	79.819	44.124	15.156	1.00 31.2			0
MOTA	2374	CB			447	77.088	42.889	13.763	1.00 30.7			C
ATOM	2375	CG1	VAL	A	447	77.151	42.519	15.235	1.00 30.2	1		С

MOTA	2376		VAL			75.705	43.416	13.424		30.13			C
ATOM	2377	N	GLU			80.228	42.679	13.490	1.00	31.79			N
ATOM	2378	CA	GLU	Α	448	81.493	42.260	14.071	1.00	32.87			С
MOTA	2379	С	GLU	Α	448	82.509	43.398	14.062	1.00	32.19			С
ATOM	2380	0	GLU	Α	448	83.329	43.506	14.970	1.00	31.93			0
ATOM	2381	CB	GLU	Α	448	82.037	41.021	13.339		34.51			С
ATOM	2382	CG	GLU			81.008	39.886	13.264		37.38			C
ATOM	2383	CD	GLU			81.609	38.522	12.933		39.91			C
ATOM	2384	OE1	GLU			82.543	38.447	12.098		41.39			0
ATOM	2385		GLU										
						81.129	37.514	13.501		40.50			0
ATOM	2386	N	ALA			82.448	44.254	13.049		31.62			N
MOTA	2387	CA	ALĄ			83.366	45.385	12.978		30.96			С
ATOM	2388	C	ALA			82.995	46.398	14.063		30.59			С
MOTA	2389	0	ALA	A	449	83.866	46.907	14.775	1.00	29.96			0
MOTA	23.90	CB	ALA	Α	449	83.304	46.040	11.600	1.00	31.10			С
MOTA	2391	N	SER	Α	450	81.701	46.686	14.187	1.00	30.07			N
ATOM	2392	CA	SER	Α	450	81.222	47.625	15.197	1.00	29.77			C
MOTA	2393	С	SER	Α	450	81.589	47.160	16.606	1.00	29.70			C
MOTA	2394	0	SER	Α	450	82.085	47.943.	17.419		29.34			0
ATOM	2395	СВ	SER			79.699	47.779	15.117		29.51			Ċ
ATOM	2396	OG	SER			79.306	48.434	13.931		29.55			Ō
ATOM	2397	N	LEU			81.341	45.884	16.886		29.59			N
ATOM	2398	CA	LEU			81.624							
							45.321	18.202		29.99			C
ATOM	2399	C	LEU			83.111	45.175	18.505		30.55			C
ATOM	2400	0	LEU			83.509	45.213	19.670		30.21		•	0
MOTA	2401	CB	LEU			80.902	43.981	18.372		28.74			C
MOTA	2402	CG	LEU			79.374	44.128	18.335		28.52			C
MOTA	2403	CD1	LEU			78.726	42.808	18.674	1.00	27.60			С
MOTA	2404	CD2	LEU	Α	451.	78.924	45.215	19.319	1.00	27.59			C
MOTA	2405	N	ASN	Α	452	83.933	45.012	17.471	1.00	31.38	•		N
MOTA	2406	CA	ASN	Α	452	85.372	44.923	17.694	1.00	32.50			C
MOTA	2407	С	ASN-	Α	452	85.838	46.287	18.185	1.00	32.25			С
MOTA	2408	0	ASN	Α	452	86.751	46.390	19.005		32.13			0
ATOM	2409	СВ	ASN		,	86.130	44.568	16.411		33.77			C
MOTA	2410	CG	ASN			86.149	43.079	16.140		36.12			C
ATOM	2411		ASN			86.254	42.263	17.066		37.33			0
ATOM	2412		ASN			86.069	42.712	14.866		37.13			N
ATOM	2413	N	LYS			85.203	47.335	17.674		31.85			N
			LYS										
ATOM	2414	CA					48.693	18.067		32.30			C
ATOM	2415	C	LYS			85.137	48.922	19.519		31.23			C
ATOM	2416	0	LYS			85.888	49.497	20.303		30.82			0
ATOM	2417	CB	LYS			84.838	49.694	17.157		33.75			С
ATOM	2418	CG	LYS			85.166	51.143	17.450	1.00	36.50			C
MOTA	2419	CD	LYS			84.539	52.063	16.406		39.06			С
MOTA	2420	CE	LYS			85.055	51.754	14.999	1.00	39.28			С
MOTA	2421	NZ	LYS	Α	453	84.355	52.589	13.978	1.00	40.79	•		N
ATOM	2422	N	VAL	Α	454	83.937	48.462	19.864	1.00	30.16			N
ATOM	2423	CA	VAL	Α	454	83.418	48.591	21.215		29.31			C
ATOM	2424	С	VAL			84.334	47.848	22.189		29.13			С
ATOM	2425	0	VAL			84.696	48.372	23.243		28.31			0
ATOM	2426	CB	VAL			81.984	48.012	21.314		29.18			C
ATOM	2427		VAL			81.506	48.019	22.765		28.54			C
MOTA	2427		VAL										C
ATOM						81.038	48.830	20.444		28.30			
	2429	N	LYS			84.705	46.623	21.824		28.92			N
MOTA	2430	CA	LYS			85.581	45.804	22.656		28.73			С
ATOM	2431	C	LYS			86.919	46.498	22.855		28.34			C
ATOM	2432	0	LYS	A	455	87.462	46.522	23.954	1.00	28.12			0
	-												

ATOM	2433	СВ	LYS	A	455		85.822	44.440	22.006	1.00 28.84	С
MOTA	2434	CG	LYS	А	455		84.620	43.517	21.976	1.00 29.31	C
ATOM	2435	CD	LYS	Α	455		84.971	42.252	21.200	1.00 29.86	C
MOTA	2436	CE	LYS	A	455		83.802	41.296	21.114	1.00 31.18	C
MOTA	2437	NZ	LYS	Α	455		84.174	40.040	20.399	1.00 31.56	N
ATOM	2438	N	SER	A	456		87.448	47.057	21.774	1.00 28.04	N
MOTA	2439	CA	SER	Α	456		88.720	47.754	21.834	1.00 28.45	C
MOTA	2440	С	SER	Α	456		88.631	48.936	22.802	1.00 27.62	C
MOTA	2441	0	SER	А	456		89.497	49.121	23.658	1.00 27.05	0
ATOM	2442	CB	SER	А	456		89.114	48.237	20.434	1.00 28.94	C
MOTA	2443	OG	SER	Α	456		90.336	48.950	20.475	1.00 31.01	0
MOTA	2444	N	THR	А	457		87.578	49.733	22.662	1.00 26.61	N
MOTA	2445	CA	THR	A	457		87.377	50.885	23.528	1.00 26.30	C
MOTA	2446	C	THR	Α	457		87.186	50.444	24.978	1.00 25.88	C
ATOM	2447	0			457	. •	87.697	51.080	25.896	1.00 25.21	0
MOTA	2448 .	CB	THR	A	457		86.157	51.706	23.070	1.00 26.38	С
MOTA	2449	OG1	THR	Α	457		86.378	52.139	21.727	1.00 27.27	0
ATOM	2450	CG2			457		85.949	52.926	23.961	1.00 25.15	C
	2451	N			458		86.456	49.353	25.184	1.00 25.53	N
MOTA	2452	CA	MET				86.244	48.857	26.535	1.00 26.03	C
MOTA	2453	С	MET				87.578	48.547	27.201	1.00 26.68	C
ATOM	2454	0	MET				87.768	48.826	28.383	1.00 26.93	0
ATOM	2455	CB	MET				85.340	47.623	26.521	1.00 25.33	C
MOTA	2456	CG	MET				83.876	47.976	26.285	1.00 24.43	C
MOTA	2457	SD	MET				82.816	46.551	26.067	1.00 25.53	S
ATOM	2458	CE			458		82.942	45.769	27.715	1.00 24.14	C
ATOM	2459	Ñ			459		88.507	47.977	26.445	1.00 27.44	N
MOTA	2460	CA			459		89.819	47.682	27.000	1.00 28.79	C
ATOM	2461	C			459		90.578	48.968	27.351	1.00 28.24	C
MOTA	2462	0			459		91.338	48.996	28.322	1.00 27.71	0
ATOM	2463	CB			459		90.628	46.819	26.030	1.00 31.37	C
MOTA	2464	SG			459		90.257	45.047	26.230	1.00 35:38	S
MOTA MOTA	2465 2466	N	ASN ASN				90.375	50.030	26.569	1.00 27.55	N
MOTA	2467	CA C	ASN				91.028	51.309	26.855	1.00 27.53	C
ATOM	2468	0	ASN				90.504 91.202	51.804 52.496	28.202 28.938	1.00 27.21 1.00 26.69	C 0
ATOM	2469	CB	ASN				90.696	52.362	25.787	1.00 20.09	C
MOTA	2470	CG	ASN				91.419	52.122	24.471	1.00 27.34	C
MOTA	2471				460		90.796	52.061	23.409	1.00 29.27	0
ATOM	2472		ASN			·	92.741	51.998	24.533	1.00 29.42	N
ATOM	2473	N			461		89.261	51.441	28.512	1.00 26.99	N
ATOM	2474	CA			461		88.632	51.855	29.755	1.00 26.90	C
ATOM	2475	C			461		88.865	50.838	30.871	1.00 26.66	C
ATOM	2476	0			461		88.367	51.003	31.976	1.00 26.77	Ö
MOTA	2477	СВ	CYS				87.126	52,063	29.538	1.00 27.30	C
ATOM	2478	SG			461		86.714	53.341	28.304	1.00 27.83	s
MOTA		N			462		89.627	49.793	30.570	1.00 26.92	N
ATOM	2480	CA			462		89.919	48.768	31.557	1.00 26.65	C
MOTA	2481	C			462		88.758	47.842	31.881	1.00 26.78	C
ATOM	2482	0	GLY				88.659	47.347	33.001	1.00 26.85	0
ATOM	2483	N			463		87.882	47.592	30.913	1.00 26.47	N
MOTA	2484	CA	ALA				86.731	46.725	31.155	1.00 26.74	С
MOTA	2485	С	ALA				86.700	45.507	30.249	1.00 26.80	С
MOTA	2486	0	ALA				86.898	45.616	29.034	1.00 26.39	0
ATOM	2487	CB	ALA				85.433	47.515	30.991	1.00 26.14	C
MOTA	2488	N	LEU	A	464		86.444	44.349	30.850	1.00 27.16	N
MOTA	2489	CA	LEU	A	464		86.356	43.101	30.105	1.00 27.87	C

MOTA	2490	С	LEU	A	464	84.901	42.683	29.943	1.00	27.47	-		C
MOTA	2491	0	LEU	Α	464	84.604	41.722	29.239	1.00	28.26			0
ATOM	2492	CB	LEU	Α	464	87.138	41.984	30.806	1.00	28.54			C
ATOM	2493	CG	LEU	Α	464	88.634	41.869	30.492	1.00	29.79			C
ATOM	2494	CD1	LEU	Α	464	88.827	41.779	28.983	1.00	29.98			C
ATOM	2495	CD2	LEU	A	464	89.388	43.078	31.039	1.00	31.57	•		C
ATOM	2496	N	THR	Α	465	83.997	43.398	30.606	1.00	26.65			N
ATOM	2497	CA	THR	A	465	82.573	43.096	30.515	1.00	25.99			С
ATOM	2498	С	THR			81.786	44.391	30.567	1.00	25.84			C
ATOM	2499	0	THR			82.318	45.435	30.945	1.00	25.20			0
ATOM	2500	CB	THR	Α	465	82.077	42.229	31.688	1.00	25.98			С
ATOM	2501	OG1	THR	Α	465	82.139	42.991	32.899		25.86			0
MOTA	2502	CG2	THR			82.921	40.975	31.827		26.08			С
ATOM	2503	N	ILE			80.514	44.316	30.197		25.29			N
ATOM	2504	CA			466.	79.666	45.495	30.219		25.21			C
ATOM	2505	C	ILE			79.470	45.999	31.650		25.01			C
ATOM	2506	0	ILE			79.569	47.197	31.902		25.19			0
ATOM	2507	СВ	ILE			78.316	45.208	29.531		25.13	•		C
ATOM	2508	CG1	ILE			78.565	45.033	28.025		25.57			C
ATOM	2509	CG2	ILE			77.323	46.336	29.809		24.41			C
ATOM	2510		ILE			77.351	44.586	27.223		26.34			C
ATOM	2511	N	PRO			79.197	45.095	32.610		25.04			N
ATOM	2512	CA	PRO			79.023	45.598	33.975		24.53			C
MOTA	2512	C	PRO			80.303	46.274	34.464		24.42	•		C
ATOM	2514	0	PRO			80.256	47.287	35.155		24.42			0
	2514		PRO				44.333	34.767		24.23			C
MOTA		CB				78.686				24.74			C
ATOM	2516	CG	PRO			77.936	43.508	33.754		24.43			C
MOTA	2517	CD	PRO			78.817	43.672	32.527					
ATOM	2518	N	GLN			81.455	45.723	34.105		24.65			N C
ATOM	2519	CA	GLN			82.702	46.335	34.536		25.05			
ATOM	2520	C	GLN			82.883	47.705	33.873		25.35			C
ATOM	2521	0	GLN			83.447	48.621	34.471		25.30			0
ATOM	2522	CB	GLN			83.890	45.430	34.219		24.93			C
ATOM	2523	CG	GLN			85.207	46.019	34.668		25.22		•	C.
ATOM	2524	CD	GLN			86.347	45.017	34.648		25.10			C.
MOTA	2525	OE1	GLN			86.493	44.234	33.707		24.05			0
ATOM	2526	NE2	GLN			87.176	45.054	35.686		25.09			N
ATOM	2527	N	LEU			82.400	47.840	32.639		25.06			N
MOTA	2528	CA	LEU			82.488	49.108	31.919		24.83			C
MOTA	2529	C.	LEU			81.609	50.150	32.617		25.01			C
ATOM	2530	0	LEU			82.023	51.292	32.838		24.50			0
ATOM	2531	CB	LEU			82.010	48.932	30.476		24.41			C
MOTA	2532	CG	LEU			81.852	50.214	29.655		24.56			C
ATOM	2533		LEU			83.223	50.807	29.360		24.30			C
MOTA	2534		LEU			81.112	49.906	28.358		24.10			C
MOTA	2535	N	GLN			80.395	49.741	32:966		25.06			N
MOTA	2536	CA	GLN			79.441	50.622	33.629		25.82			C
ATOM	2537	C	GLN			79.966	51.100	34.981		26.53			C
ATOM	2538	0	GLN			79.627	52.184	35.467		26.74			0
ATOM	2539	CB	GLN			78.102	49.886	33.775		25.24			C
ATOM	2540	CG	GLN			77.455	49.646	32.406		25.04			C
MOTA	2541	CD	GLN			76.245	48.731	32.421		25.22			С
MOTA	2542		GLN			75.453	48.722	31.469		25.47			0
ATOM	2543		GLN			76.099	47.948	33.479		24.84			N
ATOM	2544	N			471	80.829	50.291	35.572		27.02			N
ATOM	2545	CA			471	81.404	50.617	36.860		27.70			C
MOTA	2546	C	SER	A	471	82.654	51.505	36.756	1.00	27.93			С

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MOTA	2547	0	SER	A	471	82.805	52.458	37.517					0
ATOM	2548	CB	SER	A	471	81.741	49.316	37.596	1.00	27.39			С
MOTA	2549	OG	SER	Α	471	82.515	49.569	38.748	1.00	29.07			0
MOTA	2550	N	LYS	Α	472	83.522	51.208	35.794	1.00	28.02			N
ATOM	2551	CA	LYS			84.785	51.935	35.630	1.00	28.71			C
ATOM	2552	C	LYS			84.851.	53.106	34.647	1.00	28.19			С
ATOM	2553	0	LYS			85.796	53.891	34.696		28.07			0
ATOM	2554	CB	LYS			85.883	50.938	35.257		29.32			C
							49.816	36.267		31.72			C
ATOM	2555	CG	LYS			86.050							C
ATOM	2556	CD	LYS			87.050	48.764	35.805		32.09			
ATOM	2557	CE	LYS			88.459	49.308	35.753		32.85			C
MOTA	2558	NZ	LYS			89.418	48.212	35.419		33.48			N
ATOM	2559	N	ALA	А	473	83.868	53.223	33.760		27.53			N
MOTA	2560	CA	ALA	А	473	83.875	54.283	32.758	1.00	27.01			C
ATOM	2561	C	ALA	Α	473	83.977	55.698	33.313	1.00	26.91			C
ATOM	2562	0	ALA	Α	473	83.341	56.049	34.309	1.00	26.92			0
ATOM	2563	CB	ALA	A	473	82.635	54.169	31.859	1.00	27.23			C
ATOM	2564	N	LYS	Α	474	84.803	56.499	32.649	1.00	26.59			N
ATOM	2565	CA	LYS			85.012	57.898	32.999	1.00	26.15			C
MOTA	2566	C	LYS			84.444	58.636	31.791		26.08			C
ATOM	2567		LYS			84.973	58.545	30.684		25.63			0.
ATOM	2568	CB	LYS			86.504	58.161	33.190		25.22			C
						87.062	57.433	34.414		25.03			C
ATOM	2569	CG	LYS							24.53			C
ATOM	2570	CD	LYS			88.530	57.064	34.245			:		C
ATOM	2571	CE	LYS			89.433	58.274	34.298		24.54			
MOTA	2572	NZ	LYS			90.837	57.870	33.996		23.96			N
MOTA	2573	N	ILE			83.348	59.350	32.011		26.24			N
ATOM	2574	CA	ILE	А	475	82.652	60.025	30.926		26.16			С
MOTA	2575	C	ILE	Α	475	82.601	61.527	31.073	1.00	26.07			C
MOTA	2576	0	ILE	Α	475	82.064	62.045	32.049	1.00	26.61		•	0
ATOM	2577	CB	ILE	Α	475	81.206	59.489	30.821	1.00	26.31			С
ATOM	2578	CG1	ILE	Α	475	81.230	57.954	30.784	1.00	26.16			C
MOTA	2579	CG2	ILE	Α	475	80.526	60.042	29.572	1.00	26.65			C
ATOM	2580	CD1	ILE	Α	475	79.853	57.299	30.764	1.00	24.83		•	C
ATOM	2581-	N			476	83.156	62.228	30.093	1.00	25.67			N
ATOM	2582	CA	THR			83.158	63.677	30.136		25.52			С
ATOM	2583	C	THR			82.290	64.288	29.056		25.76			С
ATOM	2584	0	THR			82.160	63.752	27.951		25.51			0
		CB			476	84.581	64.261	29.977		25.15			C
ATOM	2585					84.519				24.81			0
ATOM	2586	OG1			476		65.689	30.093 28.616					C
ATOM	2587	-	THR			85.168	63.897			24.56			
ATOM	2588	N			477	81.686	65.414	29.401		26.07			N
ATOM	2589	CA			477	80.869	66.159	28.467		27.01			C
MOTA	2590	С			477	81.908	66.963	27.677		27.30			C
MOTA	2591	0	LEU	A	477	82.996	67.239	28.183		26.31		,	0
ATOM	2592	CB	LEU	Α	477	79.929	67.103	29.225		27.31			С
MOTA	2593	CG	LEU	A	477	78.834	67.808	28.421	1.00	28.63			С
MOTA	2594	CD1	LEU	Α	477	77.822	66.782	27.915	1.00	28.11			С
MOTA	2595	CD2	LEU	A	477	78.148	68.842	29.303	1.00	28.70			С
ATOM	2596	N			478	81.577	67.317	26.443	1.00	27.88			N
ATOM	2597	CA			478	82.472	68.085	25.590	1.00	29.05			С
ATOM	2598	C			478	81.802	69.428	25.295		29.61			С
ATOM	2599	Ō			478	80.581	69.504	25.177		29.56			0
ATOM	2600	CB			478	82.737	67.322	24.269		29.48			C
ATOM	2601		VAL			83.643		23.368		30.38			C
ATOM	2602		VAL			83.370	65.970	24.579		29.54			C
										30.34			N
MOTA	2603	N	SER	А	479	82.596	70.484	25.183	1.00	30.34			TA

MOTA	2604	CA	SER	Α	479	82.058	71.819	24.916	1.00	31.62			С
ATOM	2605	C	SER	А	479	81.402	71.940	23.545	1.00	32.67			С
MOTA	2606	0	SER	Α	479	81.770	71.232	22.609	1.00	31.95			0
MOTA	2607	CB	SER	А	479	83.168	72.866	25.021	1.00	30.68			C
ATOM	2608	OG	SER	А	479	84.085	72.730	23.949	1.00	30.46			0
MOTA	2609	N	SER			80.442	72.858	23.437		34.86			N
MOTA	2610	CA	SER			79.729	73.110	22.183		37.33			С
MOTA	2611	С	SER			80.703	73.371	21.041		38.47			C
ATOM	2612	0	SER			80.561	72.816	19.951		38.60			0
ATOM	2613	CB	SER			78.813	74.331	22.317		37.61			C
ATOM	2614	OG	SER			77.888	74.175	23.373		39.26			0
ATOM	2615	N	VAL			81.685	74.229	21.302		40.19			N
MOTA	2616	CA	VAL			82.694	74.592	20.311		42.19			C
													C
ATOM	2617	C	VAL			83,561	73.422	19.843		43.43			
ATOM	2618	0	VAL			83.944	73.364	18.676		43.73			·O
ATOM	2619	CB	VAL			83.617	75.716	20.848		42.42			C
MOTA	2620		VAL			84.833	75.879	19.941		42.66			C
MOTA	2621		LAV			82.844	77.029	20.917		42.27			С
MOTA	2622	N	SER			83.879	72.499	20.744		44.59			N
MOTA	2623	CA	SER			84.697	71.346	20.378		46.25			С
ATOM	2624	C	SER	А	482	84.013	70.517	19.293	1.00	47.04		•	C
ATOM	2625	0	SER	Α	482	84.670	69.773	18.556	1.00	47.14			0
MOTA	2626	CB	SER	Α	482	84.943	70.448	21.594	1.00	46.49			С
MOTA	2627	OG	SER	Α	482	85.710	71.107	22.583	1.00	48.50			0
MOTA	2628	N	ILE	Α	483	82.693	70.638	19.204	1.00	47.71			N
MOTA	2629	CA	ILE	Α	483	81.934	69.876	18.219	1.00	48.77			C
ATOM	2630	С	ILE	А	483	81.656	70.687	16.952	1.00	49.17			C
MOTA	2631	0	ILE			81.552	71.931	17.042		49.53			0
MOTA	2632	CB	ILE			80.597	69.387	18.833		48.86			C
MOTA	2633	CG1				80.886	68.549	20.081		48.85			C
ATOM	2634	CG2				79.818	68.552	17.822		49.17			C
ATOM	2635	CD1				79.650	68.141	20.845		49.07			Ċ
TER	2636		ILE										-
HETATM		K			900	52.558	59.979	29.204	0.75	33.19			K
HETATM		P	XMP		602	67.402	54.842	14.904		30.34			P
HETATM		01P			602	67.002	54.789	13.486		30.72			ō
HETATM		02P			602	68.190	53.690	15.379		30.78			o
HETATM		05'	XMP		602	66.075	54.823	15.699		29.65			0
HETATM		03P			602	67.954	56.140	15.323		30.68			0
HETATM		C5.1	XMP		602	65.078	53.767	15.814		29.12			C
HETATM		C4 '	,		602	63.985		16.886		29.12			
							54.002						C
HETATM		04'			602	63.144	55.124	16.601		29.44			0
HETATM			XMP		602	61.803		17.060		29.86			C
HETATM		N9	XMP		602	60.863	55.346	15.925		30.85			N
HETATM		C4	XMP		602	60.396	56.585	15.533		31.77			С
HETATM		И3	XMP		602	60.681	57.809	16.083		32.09			N
HETATM		N1	XMP		602	59.202	58.646	14.358		32.72			N
HETATM		C2	XMP		602	60.053	58.836	15.454		33.14	•		C
HETATM		02	XMP		602	60.229	59.983	15.858		33.63			0
HETATM		C6	MP		602	58.897	57.407	13.781		32.30		,	С
HETATM		06	MP		602	58.148	57.308	12.825	1.00	33.30			0
HETATM	2655	C5	MMP		602	59.556	56.336	14.439	1.00	32.02			. C
HETATM	2656	N7	XMP		602	59.498	55.005	14.154	1.00	31.42			N
HETATM	2657	C8	XMP.		602	60.263	54.494	15.036	1.00	31.18			C
HETATM	2658	C2 1	XMP		602	61.788	53.653	17.733	1.00	29.10			С
$\mathtt{HETATM}$	2659	02 '	MMX		602	61.947	53.880	19.132		29.07			0
HETATM	2660	C3 '	XMP		602	62.943	52.927	17.024		28.77			С

TTTTTT A TOM	2661	021	VMD	600	63.388	51.798	17.768	1.00 28.12		0
HETATM		03 '		602						P
HETATM			NAD	987	50.634	53.888	20.452			
HETATM			NAD	987	49.686	52.811	20.084	1.00 70.10		0
HETATM	2664	A02	NAD	987	51.622	53.619	21.519	1.00 70.18		0
HETATM	2665	A05*	NAD	987	49.807	55.222	20.825	1.00 70.73		0
HETATM	2666	AC5*	NAD	987	48.836	55.190	21.879	1.00 71.96		C
HETATM				987	48.158	56.575	22.018	1.00 72.40		C
HETATM				987	47.053	56.406	22.993	1.00 72.62		0
HETATM				987	47.458	56.986	20.719	1.00 72.81		С
						56.491	19.587	1.00 72.01		0
HETATM				987	48.185					C
HETATM				987	46.117	56.309	20.794	1.00 72.87		
HETATM				987	46.258	54.925	20.444	1.00 72.72		0
HETATM	2673	AC1*	NAD	987	45.766	56.439	22.272	1.00 72.67		С
HETATM	2674	AN9	NAD	987	44.784	55.412	22.731	1.00 72.51	`	N
HETATM	2675	AC8	NAD	987	43.460	55.583	22.865	1.00 72.46		С
HETATM	2676	AN7	NAD	987	42.908	54.431	23.274	1.00 72.16		N
HETATM			NAD	987	43.880	53.538	23.399	1.00 72.08		C
HETATM			NAD	987	43.920	52.200	23.781	1.00 72.01		С
HETATM			NAD.	987	42.803	51.558	24.105	1.00 72.25		N
					45.108	51.553	23.810	1.00 71.86	•	N
HETATM			NAD	987						C
HETATM			NAD	987	46.241	52.179	23.476	1.00 71.78		
HETATM			NAD	987	46.228	53.462	23.105	1.00 71.90		N
HETATM	2683	AC4	NAD	987	45.069	54.157	23.059	1.00 72.20		C
HETATM	2684	03	NAD	987	51.412	54.316	19.101	1.00 69.74		0
HETATM	2685	NP	NAD	987	52.634	55.383	19.126	1.00 69.12		P
HETATM	2686	NO1	NAD	987	53.103	55.572	20.519	1.00 68.69		0
HETATM	2687	NO2	NAD	987	52.250	56.578	18.341	1.00 69.23		0
HETATM				987	53.807	54.613	18.343	1.00 69.13		0
HETATM				987	53.538	53.954		1.00 68.98		C
HETATM				987	54.844	53.577	16.381	1.00 68.78		C
						54.846	16.049	1.00 68.83		ō
HETATM				987	55.536			1.00 68.59		C
HETATM				987	55.787	52.849	17.333			
HETATM				987	56.629	51.948	16.611	1.00 68.69		0
HETATM	2694	NC2*	NAD	987	56.615	53.936	17.951	1.00 68.50		С
HETATM	2695	NO2*	NAD	987	57.896	53.435	18.333	1.00 68.13		0
HETATM	2696	NC1*	NAD	987	56.784	54.933	16.818	1.00 68.70		С
HETATM	2697	NN1	NAD	987	57.133	56.318	17.254	1.00 69.08		N
HETATM	2698	NC2	NAD	987	58.217	56.537	18.152	1.00 69.28		C
HETATM			NAD	987	58.549	57.847	18.538	1.00 69.57		С
HETATM			NAD	987	59.715		19.514	1.00 69.91	-	² C
HETATM			NAD.	987	60.134	59.245	19.712	1.00 70.20		0
HETATM			NAD	987	60.220	57.016	20.103	1.00 69.78		N
						58.929	18.030	1.00 69.34		C
HETATM			NAD	987	57.806			1.00 69.34		C
HETATM			NAD	987	56.734	58.723	17.144			
HETATM			NAD	987	56.393	57.421	16.753	1.00 69.10		C
HETATM		0	HOH	1	80.159	44.885	4.169	1.00 45.58		0
HETATM	2707	0	HOH	2	70.459	54.183	21.914	1.00 24.31		0
HETATM	2708	0	ĤОН	3	57.313	58.461	28.306	1.00 24.50		0
HETATM	2709	0	HOH	. 4	65.571	60.118	.24.639	1.00 23.07		0
HETATM		0	нон	5	40.291	38.852	28.760	1.00 49.15		0
HETATM		0	нон	6	66.287	47.668	38.747	1.00 21.93		0
HETATM		0	нон	7	86.808	55.200	31.125	1.00 27.24		0
HETATM		0	нон	8	79.324	41.691	29.401	1.00 21.83		ō
						61.415	38.396	1.00 21.03		0
HETATM		0	HOH	9	69.419					0
HETATM		0	нон	10	58.291	50.786	22.925	1.00 24.55		
HETATM			нон	11	70.499	53.076	14.172	1.00 25.36		0
HETATM	2717	0	HOH	12	75.758	43.567	30.918	1.00 21.79		0

HETATM	2718	0	HOH	13	88.069	53.459	33.173	1.00	26.13		0
HETATM	2719	0	HOH	14	67.647	38.078	46.052	1.00	35.25		0
HETATM	2720	0	HOH	15 ,	72.291	37.808	33.719	1.00	27.23		0
HETATM	2721	0	НОН	16 .	56.445	78.452	34.278	1.00	24.45		0
HETATM	2722	0	HOH	17	58.982	44.997	36.851	1.00	25.40		O
HETATM	2723	0	НОН	18	51.923	53.605	25.905	1.00	30.95		0
HETATM		0	нон	19	58.261	35.282	26.925	1.00	32.59		0
HETATM	2725	0	нон	20	78.214	47.801	37.366		36.04		0
HETATM		0	нон	21	77.272	53.707	34.316		27.76		0
HETATM		0	НОН	22	47.841	54.106	36.571		37.78		0
HETATM		0	НОН	23	64.271	41.030	7.745		31.98		ō
HETATM		0	нон	24	73.286	57.144	36.094		24.02		0
HETATM		0	нон	25	67.036	59.452	38.278		48.34		0
HETATM		0	НОН	26	56.058	41.046	37.332		41.47		0
HETATM		0	нон	27	59.588	50.684	20.017		32.62		0
HETATM		0	нон	28	68.814	67.431	32.848		28.56		0
HETATM	-	0		29							
			НОН		81.923	66.876	31.746		32.25		0
HETATM		0	НОН	30	61.989	38.331	33.948		24.11		0
HETATM		0	HOH	31	69.891	33.131 .			33.89		0
HETATM		0	нон	32	60.032	39.147	6.730	-	39.28		0
HETATM		0	HOH	33	61,745	63.891	35.416		31.28		0
HETATM		0	НОН	34	48.981	43.802	20.915		29.86		0
HETATM		0	НОН	35	69.168	35.704	7.655		35.67		0
HETATM		0	HOH	36	76.202	65.130	31.664		44.93		0
HETATM		0	нон	37	69.263	32.519	38.368		38.37		0
HETATM		0	HOH	38	65.179	36.434	34.852	1.00	29.61		0
HETATM	2744	0	HOH	39	59.293	59.263	30.587	1.00	36.96		0
HETATM	2745	0	HOH	40	49.423	42.410	7.845	1.00	53.80		0
HETATM	2746	0	HOH	41	64.358	73.055 ·	32.790	1.00	26.48		0
HETATM	2747	0	HOH	42	71.857	63.707	34.068	1.00	60.77		0
HETATM	2748	0	HOH	43	56.071	57.344	38.813	1.00	42.44		0
HETATM	2749	0	HOH	44	63.542	56.163	20.268	1.00	36.97		0
HETATM	2750	0	HOH	45	61.356	50.051	17.813	1.00	26.22		0
HETATM	2751	0	HOH	46	92.220	40.526	20.299	1.00	49.10	,	0
HETATM	2752	0	HOH	47	71.972	61.198	21.121	1.00	35.90		0
HETATM	2753	0	HOH	48	83.870	52.797	20.905	1.00	29.24		0
HETATM	2754	0	HOH	49	56.116	76.920	37.019	1.00	36.67		0
HETATM	2755	0	НОН	50	50.418	45.939	35.861		36.94		0
HETATM	2756	Ò.	нон	51	81.571	63.014	21.227		32.08		0
HETATM		0	нон	52	66.576	33.997	36.818		42.85		0
HETATM	2758	0	НОН	53	59.306	51.362	16.242		31.71		0
HETATM		0	нон	54	58.726	37.969	34.720		37.12		0
HETATM		0	НОН	55	59.306	53.739	20.688		31.48		0
HETATM		0	НОН	56	52.755	51.235	37.729		38.98		ō
HETATM		0	НОН	57	77.948	70.194	25.195		40.94		Ō
HETATM		0	НОН	58	42.877	43.465	23.430		37.12		o
HETATM		0	нон	59	74.941	70.159	31.554		37.95		o
HETATM		0	нон	60	62.836	39.227	5.777		41.89		Ö
HETATM		0	нон	61	63.043	31.312	25.273		42.37		0
HETATM		0	НОН	62	73.944	59.700	37.703		39.09		0
HETATM		0	нон	63	45.718	48.708	27.281		38.46		
HETATM						37.356					0
		0	HOH	64	65.979		16.650		29.39		0
HETATM		0	HOH	65	74.924	38.483	8.198		36.88		0
HETATM		0	HOH	66 67	72.792	32.939	26.042		49.82		0
HETATM		0	HOH	67	71.174	32.495	29.960		43.86		0
HETATM		0	HOH	68	86.835	69.123	23.909		40.67		0
HETATM	2//4	0	НОН	69	51.919	29.585	14.737	1.00	50.08		0

					~						
HETATM	2775	0 .	нон .	70	74.502	36.683	10.729	1.00	38.28		0
HETATM	2776	0	НОН	71	74.398	47.611	35.605	1.00	39.16		0
HETATM	2777	0	НОН	72	73.613	50.462	36.144	1.00	32.41		0
HETATM	2778	0	НОН	73	54.489	46.459	17.581	1.00	46.38		0
HETATM		0	нон	74	73.145	64.449	30.898		37.64		0
HETATM		0	нон	75	69.890	53.682	17.707		40.51		0
HETATM		0	НОН	76	44.394	42.781	15.412		49.08		Ō
HETATM		0	нон	77	59.413	50.782	9.634		33.53		ō
HETATM		Ō	нон	78	68.121	74.231	33.089		42.30		Ö
HETATM		ō	нон	79	58.561	44.690	5.902		40.98		Ö
HETATM		0	нон	80	65.000	31.161	29.173		52.37		0
HETATM		0	нон	81	74.095	34.670	40.190		36.19		0
HETATM		0	нон	82	78.806	36.429	24.680		48.73		0
HETATM		0	нон	83	72.866	40.403	41.762		43.72		0
HETATM			HOH	84 .	71.162	55.709	41.762		30.47		0
HETATM			HOH						46.81		0
		0		85	50.170	31.463	16.442				
HETATM		0	HOH	86	55.811	30.709	8.794		49.33		0
HETATM		0.	нон	87	61.016	73.187	39.258		46.28		0
HETATM	•	0.	HOH	88	83.287	41.191	17.129		48.85		0
HETATM			нон	,89	85.733	38.892	22.703		43.02		0
HETATM		0	нон	90	67.617	53.275	46.890		44.36		0
HETATM		0	НОН	91	76.440		6.407		60.32		.0
HETATM		0	HOH	92	74.688	38.584	30.945		34.79		0
HETATM		0	HOH	93	57.076	65.531	38.139		47.34		0
HETATM		0	HOH	94	78.761	38.342	17.426		41.15		0
HETATM		0	HOH	95	61.259	33.096	26.930	1.00	44.33		0
HETATM		0	HOH	96	65.482	28.592	14.900		41.37		0
HETATM		0	HOH	97	93.557	52.441	21.951	1.00	58.36		Ο.
HETATM	2803	0	HOH	98	52.048	50.238	18.507	1.00	50.58		0
HETATM	2804	0	HOH	99	69.144	44.907	46.298	1.00	41.41		0
HETATM	2805	0	HOH	100	92.572	46.733	19.480	1.00	53.29		0
HETATM	2806	0	HOH	101	60.394	50.886	46.427	1.00	58.13		0
HETATM	2807	0	HOH	102	60.206	29.776	22.560	1.00	51.85		0
HETATM	2808	0	HOH	103	55.550	45.667	5.832	1.00	54.36		0
HETATM	2809	0	HOH	104	66.124	45.356	49.309	1.00	55.34		0
HETATM	2810	0	HOH	105	42.594	47.628	27.697	1.00	57.72		0
HETATM	2811	0	HOH	106	78.097	71.838	27.740	1.00	51.84		0
HETATM	2812	0	HOH	107	74.276	62.445	19.161	1.00	40.85		0
HETATM	2813	0	HOH	108	47.828	41.389	36.858	1.00	50.41		0
HETATM	2814	o .	HOH .	109	71.642	67.017	32.073	1.00	37.86		0
HETATM	2815	0	нон	110	74.696	67.506	33.229	1.00	57.41		0
HETATM	2816	0	HOH	111	75.703	52.363	36.244	1.00	30.66		0
HETATM	2817	0	HOH	112	73.719	66.099	18.701	1.00	56.53		0
HETATM	2818	0	нон	113	51.821	45.822	7.467	1.00	52.27	•	0
HETATM	2819	0	нон	114	81.307	38.594	20.656	1.00	70.73		0
HETATM	2820	0	нон	115	81.169	38.251	23.961		41.30		0
HETATM		0	HOH .	116	45.113	41.184	12.778		63.00		0
HETATM	2822	0	нон	117	68.809	39.136	48.780		38.97		0
HETATM	2823	0	НОН	118	62.055	33.092	29.952		52.24		0
HETATM		Ó	нон	119	51.760	31.011	12.019		58.64		. 0
HETATM		Ō	нон	120	59.767	32.566	33.591		52.66		0
HETATM		Ö	нон	121	56.985	32.023	26.849		57.15		0
HETATM		0	нон	122	60.737	40.820	44.361		56.30		0
HETATM		0	нон	123	64.564	25.631	14.455		43.27		0
HETATM		0	нон	124	49.818	53.007	23.891		49.86		0
HETATM		0	нон	125	50.978	50.308	21.539		35.65		0
HETATM		0	нон		67.755	31.430	25.861		55.46		0
uerwill	2031	U	non	126	07.755	21.430	23.001	1.00	25.40		U

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      HETATM 2847
      O
      HOH
      142
      74.170
      42.608
      43.856
      1.00
      52.82

      HETATM 2848
      O
      HOH
      143
      53.514
      41.420
      6.894
      1.00
      48.12

      HETATM 2849
      O
      HOH
      144
      76.967
      51.935
      3.952
      1.00
      54.45

      HETATM 2850
      O
      HOH
      145
      82.602
      55.478
      15.958
      1.00
      37.47

      HETATM 2851
      O
      HOH
      146
      58.199
      49.374
      44.387
      1.00
      54.43

                                                                                                                                    0
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   HETATM 2852 O HOH 147.
                                                        53.891 73.194 38.807 1.00 45.80
                                                                                                                                    0
   HETATM 2853 O HOH 148
                                                       48.842 61.463 23.357 1.00 44.65
                                                                                                                                    0
   HETATM 2854 O HOH 149 49.731 59.561 25.854 1.00 55.20
   HETATM 2854 O HOH 149 49.731 59.561 25.854 1.00 55.20
HETATM 2855 O HOH 150 51.048 56.764 24.880 1.00 58.92
HETATM 2856 O HOH 151 52.529 57.301 22.316 1.00 49.02
HETATM 2857 O HOH 152 46.169 58.096 27.292 1.00 44.50
HETATM 2858 O HOH 153 40.023 51.519 24.080 1.00 57.09
HETATM 2859 O HOH 154 70.783 28.023 10.528 1.00 65.20
HETATM 2860 O HOH 155 55.358 44.178 39.610 1.00 55.31
HETATM 2861 O HOH 156 50.499 52.835 39.274 1.00 56.09
HETATM 2863 O HOH 157 51.427 49.112 39.630 1.00 50.88
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  HETATM 2860 O HOH
                                                                                                                                    0
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   HETATM 2863 O HOH 158
                                                     54.238 33.150 37.602 1.00 49.72
   HETATM 2864 O HOH 159
                                                     62.155 53.228 -3.383 1.00 55.20
                                                                                                                                    0
                                                      65.352 58.405 21.237 1.00 40.73
   HETATM 2865 O - HOH 160
                                                                                                                                   0
   HETATM 2866 O HOH 161 55.476 50.398 2.549 1.00 58.50
                                                                                                                                    0
   HETATM 2867 O HOH 162 73.645 34.699 8.566 1.00 52.83
HETATM 2868 O HOH 163 71.990 36.204 6.534 1.00 56.54
HETATM 2869 O HOH 164 70.553 26.585 7.610 1.00 59.27
                                                                                                                                    0
   CONECT 202 2464
   CONECT 2464 202
   CONECT 2638 2639 2640 2641 2642
   CONECT 2639 2638
   CONECT 2640 2638
   CONECT 2641 2638 2643
   CONECT 2642 2638
   CONECT 2643 2641 2644
   CONECT 2644 2643 2645 2660
   CONECT 2645 2644 2646
   CONECT 2646 2645 2647 2658
   CONECT 2647 2646 2648 2657
   CONECT 2648 2647 2649 2655
   CONECT 2649 2648 2651
   CONECT 2650 2651 2653
   CONECT 2651 2649 2650 2652
   CONECT 2652 2651
   CONECT 2653 2650 2654 2655
   CONECT 2654 2653
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CONECT 2655 2648 2653 2656
CONECT 2656 2655 2657
CONECT 2657 2647 2656 ·
CONECT 2658 2646 2659 2660
CONECT 2659 2658
CONECT 2660 2644 2658 2661
CONECT 2661 2660
CONECT 2662 2663 2664 2665 2684
CONECT 2663 2662
CONECT 2664 2662
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CONECT 2666 2665 2667
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CONECT 2668 2667 2673
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 CONECT 2697 2696 2698 2705
 CONECT 2698 2697 2699
 CONECT 2699 2698 2700 2703
 CONECT 2700 2699 2701 2702
 CONECT 2701 2700
 CONECT 2702 2700
 CONECT 2703 2699 2704
 CONECT 2704 2703 2705
 CONECT 2705 2697 2704
                                                            70
                                                                  39
                                              6 2868 1
 MASTER 527 0 3 13
                               18
                                          0
 END
 Figure 14
 P-UC 5440
 Page 36
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OXIDOREDUCTASE
                                                  08-AUG-02
                                                              1ME7
HEADER
TITLE
          INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
TITLE
         2 TRITRICHOMONAS FOETUS WITH RVP AND MOA BOUND
COMPND
        MOL ID: 1;
COMPND
         2 MOLECULE: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE;
         3 CHAIN: A;
COMPND
COMPND
         4 SYNONYM: IMP DEHYDROGENASE, IMPDH;
COMPND
         5 EC: 1.1.1.205;
COMPND
        6 ENGINEERED: YES
SOURCE.
         MOL ID: 1;
SOURCE
         2 ORGANISM SCIENTIFIC: TRITRICHOMONAS FOETUS;
SOURCE
         3 GENE: IMPDH;
SOURCE 4 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE 5 EXPRESSION_SYSTEM_COMMON: BACTERIA;
        6 EXPRESSION SYSTEM STRAIN: H712;
SOURCE
        7 EXPRESSION SYSTEM VECTOR TYPE: PLASMID;
SOURCE
        8 EXPRESSION SYSTEM PLASMID: PBACE
SOURCE
        ALPHA BETA BARREL
KEYWDS
        X-RAY DIFFRACTION
EXPDTA
AUTHOR
          G.L.PROSISE, J.WU, H.LUECKE
JRNL
            AUTH
                  G.L.PROSISE, J.WU, H.LUECKE
                   CRYSTAL STRUCTURE OF T. FOETUS INOSINE
JRNL
JRNL
            TITL 2 MONOPHOSPHATE DEHYDROGENASE IN COMPLEX WITH THE
            TITL 3 INHIBITOR RIBAVIRIN REVEALS A CATALYSIS-DEPENDENT
JRNL
JRNL
            TITL 4 ION BINDING SITE
JRNL
            REF
                   TO BE PUBLISHED
JRNL
            REFN
REMARK
         1
REMARK
         2 RESOLUTION. 2.15 ANGSTROMS.
REMARK
REMARK
REMARK
         3 REFINEMENT.
                        : CNS 1.1
REMARK
             PROGRAM
                       : BRUNGER, ADAMS, CLORE, DELANO, GROS, GROSSE-
REMARK
             AUTHORS
         3
REMARK
                         : KUNSTLEVE, JIANG, KUSZEWSKI, NILGES, PANNU,
REMARK
                         : READ, RICE, SIMONSON, WARREN
REMARK 3
REMARK
            REFINEMENT TARGET : ENGH & HUBER
REMARK
REMARK
            DATA USED IN REFINEMENT.
REMARK
             RESOLUTION RANGE HIGH (ANGSTROMS) : 2.15
REMARK
             RESOLUTION RANGE LOW (ANGSTROMS): 49.04
                                    (SIGMA(F)) : 0.000
REMARK
             DATA CUTOFF
             OUTLIER CUTOFF HIGH (RMS(ABS(F))) : NULL
REMARK
         3
REMARK
         3
             COMPLETENESS (WORKING+TEST) (%): 94.0
REMARK
             NUMBER OF REFLECTIONS
REMARK
         3
            FIT TO DATA USED IN REFINEMENT.
REMARK
         3
REMARK
            CROSS-VALIDATION METHOD
                                              : THROUGHOUT
REMARK
            FREE R VALUE TEST SET SELECTION : RANDOM
REMARK
            R VALUE
                                (WORKING SET) : 0.233
REMARK
            FREE R VALUE
                                              : 0.264
REMARK
         3 . FREE R VALUE TEST SET SIZE
                                          (%): 5.200
            FREE R VALUE TEST SET COUNT
REMARK
         3
                                              : 1712
             ESTIMATED ERROR OF FREE R VALUE : 0.006
REMARK
REMARK
REMARK
        3 FIT IN THE HIGHEST RESOLUTION BIN.
```

```
REMARK 3 TOTAL NUMBER OF BINS USED
REMARK 3 BIN RESOLUTION RANGE HIGH
                                       (A) : 2.15
REMARK 3 BIN RESOLUTION RANGE LOW (A): 2.28
REMARK
       3 BIN COMPLETENESS (WORKING+TEST) (%): 77.30
REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 4218
REMARK 3 BIN R VALUE (WORKING SET) : 0.288
                               (WORKING SET) : 0.2880
                                            : 0.3290
REMARK 3 BIN FREE R VALUE
REMARK 3 BIN FREE R VALUE TEST SET SIZE (%): 4.80
REMARK 3 BIN FREE R VALUE TEST SET COUNT : 215
REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.023
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 2782
REMARK 3 NUCLEIC ACID ATOMS
                                 : 0
                              : 46
: 120
REMARK 3 HETEROGEN ATOMS
REMARK 3 SOLVENT ATOMS
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2): 33.10
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 44.70
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : 0.00000
REMARK 3 B22 (A**2) : 0.00000
REMARK 3 B33 (A**2) : 0.00000
REMARK 3 B12 (A**2): 0.00000
REMARK 3 B13 (A**2) : 0.00000
REMARK 3 B23 (A**2): 0.00000
REMARK 3
REMARK 3 ESD FROM LUZZATI PLOT (A): 0.29
REMARK 3 ESD FROM SIGMAA (A): 0.25
REMARK 3 LOW RESOLUTION CUTOFF (A): 5.00
REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT (A) : 0.35
REMARK 3 ESD FROM C-V SIGMAA
                                     (A) : 0.28
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS (A): 0.006
REMARK
        3 BOND ANGLES
                               (DEGREES) : 1.20
REMARK
                               (DEGREES) : 22.50
        3 DIHEDRAL ANGLES
REMARK 3 IMPROPER ANGLES
                               (DEGREES) : 0.71
REMARK 3
        3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK
REMARK
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                              RMS
REMARK 3 MAIN-CHAIN BOND (A**2): 1.190; 1.500
REMARK 3 MAIN-CHAIN ANGLE
                                     (A**2) : 2.070 ; 2.000
REMARK 3 SIDE-CHAIN BOND
                                     (A**2) : 1.630 ; 2.000
REMARK 3 SIDE-CHAIN ANGLE
                                     (A**2) : 2.500 ; 2.500
REMARK 3
REMARK 3 BULK SOLVENT MODELING:
REMARK 3 METHOD USED : FLAT MODEL
REMARK 3 KSOL : 0.36
REMARK 3 BSOL
                      : 41.54
REMARK 3
REMARK 3 NCS MODEL : NULL
```

```
REMARK 3
REMARK 3 NCS RESTRAINTS.
                                                       RMS SIGMA/WEIGHT
REMARK 3 GROUP 1 POSITIONAL (A): NULL; NULL
REMARK 3 GROUP 1 B-FACTOR (A**2): NULL; NULL
REMARK 3
REMARK 3 PARAMETER FILE 1 : PROTEIN REP.PARAM
REMARK 3 PARAMETER FILE 2 : PARAM.GNSOL
REMARK 3 PARAMETER FILE 3 : CIS PEPTIDE. PARAM
REMARK 3 PARAMETER FILE 4 : RMP MPA.PAR
REMARK 3 PARAMETER FILE 4 : RMP_MPA.FAR
REMARK 3 PARAMETER FILE 5 : ION.PARAM
REMARK 3 PARAMETER FILE 6 : NULL
REMARK 3 TOPOLOGY FILE 1 : PROTEIN.TOP
REMARK 3 TOPOLOGY FILE 2 : RMP.TOP
REMARK 3 TOPOLOGY FILE 3 : MPA.TOP
REMARK 3 TOPOLOGY FILE 4 : ION.TOP
REMARK 3 TOPOLOGY FILE 5 : TOPH.GNSOL
REMARK 3 TOPOLOGY FILE 6 : NULL
REMARK . 3
REMARK 3 OTHER REFINEMENT REMARKS: NULL
REMARK 4
REMARK 4 1ME7 COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 16-AUG-2002.
REMARK 100 THE RCSB ID CODE IS RCSB016849.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE
                                            : X-RAY DIFFRACTION
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFR.
REMARK 200 DATE OF DATA COLLECTION : 12-JUN-2001
REMARK 200 TEMPERATURE (KELVIN) : 100.0
REMARK 200 PH
                                            : 7.50
REMARK 200 NUMBER OF CRYSTALS USED
REMARK 200
REMARK 200 SYNCHROTRON
                               (Y/N) : Y
: SSRL
REMARK 200 RADIATION SOURCE
REMARK 200 BEAMLINE
                                            : 9-1
REMARK 200 BEAMLINE : 9-1
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE
                                      (A) : 0.97
 REMARK 200 MONOCHROMATOR
                                        : NULL
REMARK 200 OPTICS
                                             : NULL
REMARK 200
REMARK 200 DETECTOR TYPE
                                            : IMAGE PLATE
REMARK 200 DETECTOR MANUFACTURER : MARRESEARCH
 REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE : SCALEPACK
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 33143
REMARK 200 RESOLUTION RANGE HIGH (A): 2.150
REMARK 200 RESOLUTION RANGE LOW (A): 50.000
 REMARK 200 REJECTION CRITERIA (SIGMA(I)) : 0.000
REMARK 200
 REMARK 200 OVERALL.
                                        (%) : 94.0
 REMARK 200 COMPLETENESS FOR RANGE
REMARK 200 DATA REDUNDANCY
                                          : 5.300
REMARK 200 R MERGE
                                         (I) : 0.07200
REMARK 200 R SYM
                                         (I) : NULL
REMARK 200 <1/SIGMA(I) > FOR THE DATA SET : 2.0500
```

```
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.15
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.19
REMARK 200 COMPLETENESS FOR SHELL (%): 79.5
REMARK 200 DATA REDUNDANCY IN SHELL : NULL
REMARK 200 R MERGE FOR SHELL (I): 0.49100
REMARK 200 R SYM FOR SHELL (I): NULL
REMARK 200 <I/SIGMA(I) > FOR SHELL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: FOURIER SYNTHESIS
REMARK 200 SOFTWARE USED: CNS
REMARK 200 STARTING MODEL: PDB ENTRY 1AK5
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: SODIUM MALONATE, TRIS, 2-
REMARK 280 MERCAPTOETHANOL, EDTA, GLYCEROL
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 4 3 2
REMARK 290
              SYMOP SYMMETRY
REMARK 290
              NNNMMM OPERATOR
REMARK 290
            1555 X,Y,Z
REMARK 290
REMARK 290
               2555 -X,-Y,Z
REMARK 290 3555 -X,Y,-Z
             4555 X,-Y,-Z
REMARK 290
REMARK 290
              5555 Z,X,Y
REMARK 290
               6555 Z,-X,-Y
REMARK 290
               7555 -Z,-X,Y
               8555
REMARK 290
                       -Z,X,-Y
              9555 Y,Z,X
10555 -Y,Z,-X
REMARK 290
REMARK 290
            11555 Y,-Z,-X
REMARK 290
REMARK 290 12555 -Y,-Z,X
REMARK 290 13555 Y,X,-Z
REMARK 290
              14555 -Y,-X,-Z
            15555 Y,-X,Z
REMARK 290
             16555 -Y,X,Z
17555 X,Z,-Y
REMARK 290
REMARK 290
              18555
REMARK 290
                      -X,Z,Y
             19555 -X,-Z,-Y
20555 X,-Z,Y
REMARK 290
REMARK 290
             21555 Z,Y,-X
REMARK 290
REMARK 290
              22555 Z,-Y,X
REMARK 290
             23555 -Z,Y,X
REMARK 290
              24555 -Z,-Y,-X
REMARK 290
REMARK 290
              WHERE NNN -> OPERATOR NUMBER
REMARK 290
               MMM -> TRANSLATION VECTOR
REMARK 290
```

REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY REMARK 290 RELATED MOLECULES. 1 1.000000 0.000000 0.000000 REMARK 290 SMTRY1 0.00000 REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY3 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 0.000000 -1.000000 0.000000 0.00000 2 REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 3 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 3 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY3 . 3 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY1 4 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 4 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY3 4 0.000000 0.000000 -1.000000 0.00000 5 0.000000 REMARK 290 SMTRY1 0.000000 1.000000 0.00000 REMARK 290 SMTRY2 5 1.000000 0.000000 0.000000 0.00000 5 0.000000 1.000000 0.000000 REMARK 290 SMTRY3 0.00000 REMARK 290 SMTRY1 6 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY2 6 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 6 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY1 7 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY2 7 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 7 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY1 8 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY2 8 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 8 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY1 9 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 9 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY3 9 1.000000 0.000000 0.000000 0.00000 SMTRY1 REMARK 290 10 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 10 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY3 10 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 11 0.000000 1.000000 0.000000 0.00000 REMARK 290 11 0.000000 0.000000 -1.000000 SMTRY2 0.00000 REMARK 290 11 -1.000000 0.000000 0.000000 SMTRY3 0.00000 REMARK 290 SMTRY1 12 0.000000 -1.000000 0.000000 0.00000 0.000000 0.000000 -1.000000 REMARK 290 SMTRY2 12 0.00000 REMARK 290 SMTRY3 12 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 13 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 1.000000 0.000000 0.000000 13 0.00000 REMARK 290 SMTRY3 13 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY1 14 0.000000 -1.000000 0.000000 0.00000 SMTRY2 REMARK 290 14 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 0.000000 0.000000 -1.000000 14 0.00000 REMARK 290 SMTRY1 15 0.000000 1.000000 0.000000 0.00000 REMARK 290 - SMTRY2 15 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 15 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 16 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 1.000000 0.000000 0.000000 16 0.00000 REMARK 290 SMTRY3 16 0:000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 17 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 17 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY3 17 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY1 18 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 18 0.000000 0.000000 1.000000 0.00000

```
REMARK 290
          SMTRY3 18 0.000000 1.000000 0.000000
                                                      0.00000
REMARK 290 SMTRY1 19 -1.000000 0.000000 0.000000
                                                      0.00000
          SMTRY2 24 0.000000 -1.000000 0.000000 0.000000
SMTRY3 24 -1.000000 0.000000 0.000000 0.00000
REMARK 290
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 1 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.000000
                                                   0.00000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000
REMARK 350 BIOMT1 2 -1.000000 0.000000 0.000000
                                                   155.06800
REMARK 350 BIOMT2 2 0.000000 -1.000000 0.000000 155.06800
REMARK 350 BIOMT3 2 0.000000 0.000000 1.000000
                                                    0.00000
REMARK 350
          BIOMT3 4 0.000000 0.000000 1.000000
                                                     0.00000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEO=SEOUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465
          M RES C SSSEQI
          MET A 1
REMARK 465
REMARK 465
            SER A
                    108
```

REMARK	465	ASN A	109
REMARK	465	VAL A	110
REMARK	465	LYS A	111
REMARK	465	PRO A	112
REMARK	465	ASP A	113
REMARK	465	GLN A	114
REMARK	465	THR A	115
REMARK	465	PHE A	116
REMARK	465	ALA A	117
REMARK	465	ASP A	118
REMARK	465	VAL A	119
REMARK	465	LEU A	120
REMARK	465	ALA A	121
REMARK	465	ILE A	122
REMARK	465	SER A	123
REMARK	465	GLN A	124
REMARK	465	ARG A	125
REMARK	465	THR A	126
REMARK	465	THR A	127
REMARK		HIS A	128
REMARK		ASN A	129
REMARK		THR A	130
REMARK	465	VAL A	131
REMARK	465	ALA A	132
REMARK	465	VAL A	133
REMARK		THR A	134
REMARK		ASP A	135
REMARK		ASP A	136
REMARK	465	GLY A	137
REMARK	465	THR A	138
REMARK	465	PRO A	139
REMARK	465	HIS A	140
REMARK		GLY A	141
REMARK		VAL A	142
REMARK			143
REMARK	465	LEU A LEU A	144
REMARK	465	GLY A	145
REMARK	465		
REMARK			146 147
REMARK		VAL A THR A	148
REMARK		GLN A	149
REMARK		ARG A	150
REMARK	465	ASP A	151
REMARK	465	TYR A	152
REMARK	465	PRO A	153
REMARK	465	ILE A	154
REMARK	465	ASP A	155
REMARK		LEU A	156
REMARK	465	THR A	157
REMARK	465	GLN A	158
REMARK	465	THR A	159
REMARK	465	GLU A	160
REMARK	465	THR A	161
REMARK	465	LYS A	162
REMARK	465	VAL A	163
REMARK	465	SER A	164
REMARK	465	ASP A	165

REMARK	465	MET A	166
REMARK	465	MET A	167
REMARK	465	THR A	168
REMARK	465	PRO A	169
REMARK		PHE A	170
REMARK	465	SER A	171
REMARK	465	LYS A	172
REMARK	465	LEU A	173
REMARK	465	VAL A	174
REMARK	465	THR A	175
REMARK		ALA A	176
REMARK		HIS A	177
REMARK	465	GLN A	178
REMARK	465	ASP A	179
REMARK	465	THR A	180
REMARK			
		LYS A	181
REMARK		LEU A	182
REMARK	465	SER A	183
REMARK	465	GLU A	184
REMARK	465	ALA A	185
REMARK	465	ASN A	186
REMARK		LYS A	187
REMARK	465	ILE A	188
REMARK	465	ILE A	189
REMARK	465	TRP A	190
REMARK	465	GLU A	191
REMARK	465	LYS A	192
REMARK	465	LYS A	193
REMARK	465	LEU A	194
REMARK	465	ASN A	195
REMARK	465	ALA A	196
REMARK	465	LEU A	197
REMARK		PRO A	198
REMARK	465	ILE A	199
REMARK	465	ILE A	200
REMARK	465	ASP A	201
REMARK	465	ASP A	202
REMARK		ASP A	202
REMARK		GLN A	204
REMARK			204
	465		
REMARK REMARK		LEU A	206
		ARG A	207
REMARK		TYR A	208
REMARK		ILE A	209
	465	VAL A	210
REMARK	465	PHE A	211
REMARK		ARG A	212
REMARK		LYS A	213
REMARK		ASP A	214
	465	TYR A	215
REMARK	465	ASP A	216
REMARK	465	ARG A	217
REMARK	465	SER A	218
REMARK	465	GLN A	219
REMARK	465	GLN A	417
REMARK	465	ARG A	418
REMARK	465	TYR A	419

```
REMARK 465
              ASP A
                      420
REMARK 465
              LEU A
                      421
REMARK 465
             GLY A
                      422
REMARK 465
              GLY A
                      423
REMARK 465 · LYS A
                      424
REMARK 465
              GLN A
REMARK 465
              LYS A
                      426
             LEU A
REMARK 465
                      427
              SER A
REMARK 465
                      428
             PHE A
REMARK 465
                      429
REMARK 465
              GLU A
                      430
REMARK 465
              VAL A
                      493
REMARK 465
             LYS A
                      494
REMARK 465
              ASP A
                      495
REMARK 465
              ARG A
                      496
REMARK 465
              ILE A
                      497
             ASN A
REMARK 465
                      498
REMARK 465
              ASP A
                      499
              TYR A
REMARK 465
                      500
REMARK 465
             HIS A
                      501
REMARK 465
             PRO A
                       502
REMARK 465
              LYS A
                      503
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, 2(A3, 1X, A1, I4, A1, 1X, A4, 3X), F6.3)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1
                               RES CSSEQI ATM2
                                                DEVIATION
           ASP A 107 OD2
REMARK 500
                               ASP A 107 CG
                                                  0.080
REMARK 500
             MET A 373
                         CE
                               MET A 373
                                           SD
                                                  0.038
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEO=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1
                                      ATM3
                               ATM2
REMARK 500
            GLY A 20
                        N - CA - C
                                           ANGL. DEV. = -7.6 DEGREES
                             - CA - C
REMARK 500
              ILE A 27
                         N
                                           ANGL. DEV. = -7.8 DEGREES
REMARK 500
             ILE A 52
                         N -
                                CA - C
                                          ANGL. DEV. = -7.9 DEGREES
```

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REMARK 500
             SER A 63
                               CA - C
                                          ANGL. DEV. = 8.1 DEGREES
REMARK 500
                               CA - C
                                          ANGL. DEV. = -7.5 DEGREES
             GLY A 64
                       N
                           - CA -
REMARK 500
             GLY A 305
                                     С
                                          ANGL. DEV. = 7.5 DEGREES
                        N
REMARK 500
                           - CA -
                                          ANGL. DEV. = -7.4 DEGREES
            SER A 357
                                     C
                        N
REMARK 500
                           - CA .-
                                          ANGL. DEV. = 7.7 DEGREES
             LYS A 444
                                     С
                        N
                                          ANGL. DEV. = 7.6 DEGREES
REMARK 500
             LYS A 472
                        N
                               CA
                                     C
REMARK 500
                                          ANGL. DEV. = -9.1 DEGREES
             LYS A 474
                        N
                            -
                               CA
                                   - C
REMARK 500
             LEU A 477
                        N
                               CA
                                     С
                                          ANGL. DEV. = -8.2 DEGREES
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1AK5
                            RELATED DB: PDB
REMARK 900 INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
REMARK 900 TRITRICHOMONAS FOETUS
REMARK 900 RELATED ID: 1ME8 RELATED DB: PDB
REMARK 900 1ME8 CONTAINS THE SAME PROTEIN WITH RVP BOUND
REMARK 900 RELATED ID: 1ME9 RELATED DB: PDB
REMARK 900 1ME9 CONTAINS THE SAME PROTEIN WITH IMP BOUND
REMARK 900 RELATED ID: 1MEH RELATED DB: PDB
REMARK 900 1MEH CONTAINS THE SAME PROTEIN WITH IMP AND MOA BOUND
REMARK 900 RELATED ID: 1MEI RELATED DB: PDB
REMARK 900 1MEI CONTAINS THE SAME PROTEIN WITH XMP AND MYCOPHENOLIC
REMARK 900 ACID BOUND
REMARK 900 RELATED ID: 1MEW
                            RELATED DB: PDB
REMARK 900 1MEW CONTAINS THE SAME PROTEIN WITH XMP AND NAD BOUND
DBREF 1ME7 A 1 503 SWS P50097 IMDH TRIFO 1 503
SEORES
        1 A 503 MET ALA LYS TYR TYR ASN GLU PRO CYS HIS THR PHE ASN
SEORES
        2 A 503 GLU TYR LEU LEU ILE PRO GLY LEU SER THR VAL ASP CYS
SEQRES
        3 A 503 ILE PRO SER ASN VAL ASN LEU SER THR PRO LEU VAL LYS
SEORES
        4 A 503 PHE GLN LYS GLY GLN GLN SER GLU ILE ASN LEU LYS ILE
        5 A 503 PRO LEU VAL SER ALA ILE MET GLN SER VAL SER GLY GLU
SEORES
SEORES
        6 A 503 LYS MET ALA ILE ALA LEU ALA ARG GLU GLY GLY ILE SER
SEORES
        7 A 503 PHE ILE PHE GLY SER GLN SER ILE GLU SER GLN ALA ALA
SEORES
        8 A 503 MET VAL HIS ALA VAL LYS ASN PHE LYS ALA GLY PHE VAL
SEORES
       9 A 503 VAL SER ASP SER ASN VAL LYS PRO ASP GLN THR PHE ALA
SEQRES 10 A 503 ASP VAL LEU ALA ILE SER GLN ARG THR THR HIS ASN THR
       11 A 503 VAL ALA VAL THR ASP ASP GLY THR PRO HIS GLY VAL LEU
SEORES
SEORES
       12 A 503 LEU GLY LEU VAL THR GLN ARG ASP TYR PRO ILE ASP LEU
SEQRES 13 A 503 THR GLN THR GLU THR LYS VAL SER ASP MET MET THR PRO
SEQRES 14 A 503 PHE SER LYS LEU VAL THR ALA HIS GLN ASP THR LYS LEU
SEQRES 15 A 503 SER GLU ALA ASN LYS ILE ILE TRP GLU LYS LYS LEU ASN
SEQRES 16 A 503 ALA LEU PRO ILE ILE ASP ASP GLN HIS LEU ARG TYR
SEQRES 17 A 503 ILE VAL PHE ARG LYS ASP TYR ASP ARG SER GLN VAL CYS
SEQRES 18 A 503 HIS ASN GLU LEU VAL ASP SER GLN LYS ARG TYR LEU VAL
SEQRES 19 A 503 GLY ALA GLY ILE ASN THR ARG ASP PHE ARG GLU ARG VAL
SEQRES 20 A 503 PRO ALA LEU VAL GLU ALA GLY ALA ASP VAL LEU CYS ILE
SEQRES 21 A 503 ASP SER SER ASP GLY PHE SER GLU TRP GLN LYS ILE THR
SEORES
       22 A 503
                 ILE GLY TRP ILE ARG GLU LYS TYR GLY ASP LYS VAL LYS
SEQRES 23 A 503
                 VAL GLY ALA GLY ASN ILE VAL ASP GLY GLU GLY PHE ARG
SEQRES 24 A 503
                 TYR LEU ALA ASP ALA GLY ALA ASP PHE ILE LYS ILE GLY
SEQRES 25 A 503 ILE GLY GLY GLY SER ILE CYS ILE THR ARG GLU GLN LYS
SEQRES 26 A 503 GLY ILE GLY ARG GLY GLN ALA THR ALA VAL ILE ASP VAL
SEQRES 27 A 503 VAL ALA GLU ARG ASN LYS TYR PHE GLU GLU THR GLY ILE
SEQRES 28 A 503 TYR ILE PRO VAL CYS SER ASP GLY GLY ILE VAL TYR ASP
SEQRES 29 A 503 TYR HIS MET THR LEU ALA LEU ALA MET GLY ALA ASP PHE
SEQRES 30 A 503 ILE MET LEU GLY ARG TYR PHE ALA ARG PHE GLU GLU SER
SEQRES 31 A 503 PRO THR ARG LYS VAL THR ILE ASN GLY SER VAL MET LYS
```

SEQRES 32 A 503 GLU TYR TRP GLY GLU GLY SER SER ARG ALA ARG ASN TRP

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SEORES 33 A 503 GLN ARG TYR ASP LEU GLY GLY LYS GLN LYS LEU SER PHE
 SEQRES 34 A 503 GLU GLU GLY VAL ASP SER TYR VAL PRO TYR ALA GLY LYS
 SEQRES 35 A 503 LEU LYS ASP ASN VAL GLU ALA SER LEU ASN LYS VAL LYS
 SEQRES 36 A 503 SER THR MET CYS ASN CYS GLY ALA LEU THR ILE PRO GLN
 SEQRES 37 A 503 LEU GLN SER LYS ALA LYS ILE THR LEU VAL SER SER VAL
 SEQRES 38 A 503 SER ILE VAL GLU GLY GLY ALA HIS ASP VAL ILE VAL LYS
 SEORES 39 A 503 ASP ARG ILE ASN ASP TYR HIS PRO LYS
     NA 901
                  1
       K A 900
 HET
                    1
 HET
       RVP 602
                    21
HET
      MOA 600
                    23
 HETNAM NA SODIUM ION
 HETNAM
           K POTASSIUM ION
 HETNAM
         RVP RIBAVIRIN MONOPHOSPHATE
        MOA MYCOPHENOLIC ACID
 HETNAM
 HETSYN
         MOA 6-(1,3-DIHYDRO-7-HYDROXY-5-METHOXY-4-METHYL-1-
 HETSYN 2 MOA OXOISOBENZOFURAN-6-YL)-4-METHYL-4-HEXANOIC ACID
 FORMUL 2 NA NA1 1+
 FORMUL 3 K K1 1+
 FORMUL 4 RVP C8 H13 N4 O8 P1
 FORMUL 5 MOA
               C17 H20 O6
 FORMUL 6 HOH *120 (H2 O1)
 HELIX 1 1 THR A 11 ASN A 13 5
                                                                 3
 HELIX 2 2 ILE A 27 VAL A 31 5
 HELIX 3 3 GLY A 64 GLU A 74 1
                                                                 11
 HELIX 4 4 SER A 85 ASN A
                              98 1
                                                                 14
 HELIX 5 5 ASP A 242 ALA A 253 1
                                                                 12
       6 6 SER A 267 GLY A 282 1
7 7 ASP A 283 VAL A 285 5
8 8 ASP A 294 ALA A 304 1
 HELIX
                                                                 16
 HELIX
                                                                 3
 HELIX
                                                                 1.7
 HELIX
        9 9 GLY A 330 GLY A 350 1
                                                                 21
 HELIX
       10 10 TYR A 363 MET A 373 1
                                                                 11
 HELIX 11 11 GLY A 381 ARG A 386 1
                                                                 6
 HELIX 12 12 LYS A 442 CYS A 461 1
                                                                 20
 HELIX 13 13 THR A 465 ALA A 473 1
 SHEET 1 A 2 TYR A 15 ILE A 18 0
      2 A 2 LYS A 474 LEU A 477 -1 O LYS A 474 N ILE A 18 '
 SHEET
 SHEET
      1 B 2 THR A 35 PRO A 36 0
                                                 N THR A 35
 SHEET
      2 B 2 ASN A 49 LEU A 50 -1 O LEU A 50
        1 · C 2 PHE A 40 GLN A 41 0
 SHEET
 SHEET
        2 C 2 ILE A 351 TYR A 352 -1 O TYR A 352
                                                  N PHE A 40
        1
           D 9 LEU A 54 SER A 56 0
 SHEET
        2 D 9 ILE A 77 ILE A 80 1 O ILE A 77 N SER A 56
 SHEET
                                                N ILE A 80
 SHEET
           D 9 GLY A 235 ILE A 238 1 O GLY A 237
        3
 SHEET
        4 D 9 VAL A 257 ILE A 260 1 O CYS A 259 N ILE A 238
 SHEET
       5 D 9 VAL A 287 ILE A 292 1 O GLY A 288 N LEU A 258
 SHEET
       6 D 9 PHE A 308 ILE A 311 1 O LYS A 310 N ALA A 289
 SHEET
      7 D 9 VAL A 355 ASP A 358 1 O CYS A 356 N ILE A 311
 SHEET 8 D 9 PHE A 377 LEU A 380 1 O MET A 379 N SER A 357
 SHEET 9 D 9 LEU A 54 SER A 56 1 N VAL A 55 O ILE A 378
 SHEET 1 E 3 LYS A 394 ILE A 397 0
 SHEET 2 E 3 SER A 400 TRP A 406 -1 O MET A 402 N VAL A 395
 SHEET 3 E 3 ASP A 434 PRO A 438 -1 O SER A 435 N TYR A 405
 SSBOND 1 CYS A 26 CYS A 459
                                           1.08
 CISPEP 1 GLY A 290 ASN A 291 0
 CRYST1 155.068 155.068 155.068 90.00 90.00 90.00 P 4 3 2 24
 ORIGX1 1.000000 0.000000 0.000000 0.00000
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ORIGX2		0.000	0000	1.	.000000	0.00000	0	0.00000					
ORIGX3		0.000	0000	0.	.000000	1.00000	0	0.00000					
SCALE1		0.006			.000000	0.00000	0	0.00000					
SCALE2		0.000			.006449	0.00000	0	0.00000					
SCALE3		0.000			.000000	0.00644		0.00000					
ATOM	1	N	ALA		2	55.337	75.180	36.704	1.00	34.41			N
ATOM	2	CA	ALA		2	56.037	74.068	35.999		33.40			С
ATOM	3	C	ALA		2	57.330	73.693	36.728		33.89			C
ATOM	4	0	ALA		2	57.769	74.397	37.640		32.06			0
	5	CB	ALA		2	56.344	74.482	34.569		33.59			Ç
ATOM										33.85			N
ATOM	6	N	LYS		3	57.931	72.578	36.328					C
ATOM	7	CA	LYS		3	59.175	72.132	36.943		35.52			
ATOM	8	C	LYS		3	60.319	72.311	35.953		34.41			C
ATOM	9	0	LYS		3	60.214	71.899	34.800		34.80			0
ATOM	10	CB	LYS		3	59.086	70.654	37.343		38.16			C
MOTA	11	CG	LYS		.3	60.364	70:140	38.018		42.91			C
ATOM	12	CD	LYS	A	3	60.512	68.625	37.892		46.63			C
ATOM	13	CE	LYS	А	3	61.851	68.159	38.443	1.00	48.14			C
ATOM	14	NZ	LYS	Ą	3	62.983	68.796	37.717	1.00	49.64			N
ATOM	15	N	TYR	Α	4	61.410	72.915	36.413	1.00	33.82			N
ATOM	16	CA	TYR	A	4	62.582	73.157	35.576	1.00	34.00			C
ATOM	17	С	TYR	A	4	63.792	72.378	36.094	1.00	35.31			C
ATOM	18	0	TYR	A	4	63.748	71.806	37.179	1.00	35.23			0
ATOM	19	CB	TYR	Α	4	62.886	74.661	35.548	1.00	32.00			C
MOTA	20	CG	TYR		4	61.771	75.471	34.930		31.34			С
ATOM	21		TYR		4	61.659	75.598	33.546		30.66			C
ATOM	22		TYR		4	60.793	76.070	35.726		32.52			C
ATOM	23		TYR		4	60.593	76.303	32.969		29.90			C
ATOM	24	CE2	TYR		4	59.726	76.776	35.158		30.38			C
ATOM	25	CZ	TYR		4	59.635	76.884	33.784		29.87			C
ATOM	26	OH	TYR		4 ~.	58.582	77.565	33.222		31.29			0
										36.84			
ATOM	27	N	TYR		5	64.867	72.351	35.314					N
ATOM	28	CA	TYR		5	66.072	71.630	35.708		38.47			C
ATOM	29	C	TYR		5	67.273	72.559	35.843		39.48			C
MOTA	30	0	TYR		5	67.312	73.636	35.243		39.29			0
MOTA	31	CB	TYR		5	66.377	70.519	34.698		37.98	-		C
MOTA	32	CG	TYR		5	65.243	69.530	34.551		38.25			С
MOTA	33		TYR		5	64.068	69.884	33.884		38.19			С
MOTA	34		TYR		5	65.320	68.258	35.128		37.95			С
MOTA	35		TYR	A	5	62.995	69.002	33.796	1.00	38.93			C
MOTA	36	CE2	TYR	A	5	64.251	67.363	35.050	1.00	38.15			С
MOTA	37	CZ	TYR	A	5	63.091	67.744	34.383	1.00	39.68			C
AŢOM	38	OH	TYR	A	5	62.028	66.879	34.309	1.00	38.51		•	0
MOTA	39	N	ASN	Α	6	68.249	72.136	36.641	1.00	40.42	*		N
MOTA	40	CA	ASN	·A	6	69.450	72.931	36.876	1.00	41.21			С
MOTA	41	C	ASN	A	6	70.427	72.917	35.706	1.00	40.26			С
MOTA	42	0	ASN	A	6	71.205	73.851	35.543	1.00	40.88			0
MOTA	43	CB	ASN		6	70.164	72.432	38.134		44.17			C
MOTA	44	CG	ASN		6	69.365	72.682	39.400	1.00	48.00			C
ATOM	45		ASN		6	69.468	71.926	40.371		49.62			0
ATOM	46		ASN		6	68.574	73.757	39.405		49.76			N
ATOM	47	N	GLU		7	70.388	71.868	34.892		38.65			N
ATOM	48	CA	GLU		7	70.304	71.760	33.754		37.25			C
ATOM	49	C	GLU		7	70.606	71.443	32.441		34.73			C
ATOM	50	0	GLU		· 7	69.592	70.750	32.441	•	34.73			0
		CB						34.004		34.20			C
MOTA	51		GLU		7	72.340	70.656						
ATOM	52	CG	GLU	A	7	73.284	70.878	35.186	1.00	43.43			C

ATOM	53	CD	GLU	Α	7	74.155	72.110	35.020	1.00 45.61	С
ATOM	54	OE1	GLU	A	7	74.568	72.401	33.874	1.00 45.97	0
ATOM	55	OE2	GLU	Α	7	74.438	72.779	36.040	1.00 49.17	0
MOTA	56	N	PRO	A	8	71.140	71.952	31.326	1.00 32.47	N
MOTA	57	CA	PRO	Α	8	70.498	71.644	30.048	1.00 31.28	С
ATOM	58	С	PRO	Α	8	70.855	70.188	29.731	1.00 31.10	С
MOTA	59	0	PRO	Ą	8	71.830	69.667	30.271	1.00 30.11	0
ATOM	60	CB	PRO	A	8	71.160	72.627	29.089	1.00 31.56	C
MOTA	61	CG	PRO	Α	8	72.558	72.782	29.675	1.00 30.51	С
MOTA	62	CD	PRO	A	8	72.273	72.883	31.153	1.00 32.79	C
ATOM	63	N	CYS	A	9	70.077	69.522	28.882	1.00 30.22	N
ATOM	64	CA	CYS	Α	9	70.389	68.137	28.531	1.00 29.58	C
MOTA	65	C	CYS	А	9	71.493	68.098	27.462	1.00 28.36	C
MOTA	66	0	CYS	Α	9	71.727	69.096	26.772	1.00 26.35	0
MOTA	67	CB	CYS	Α	9	69.124	67.414	28.046	1.00 31.88	C
ATOM	68	SG	CYS		9	68.260	68.177	26.653	1.00 38.35	S
MOTA	69	N	HIS	A	10	72.169	66.955	27.343	1.00 27.89	N
MOTA	70	CA	HIS	Α	10	73.271	66.765	26.391	1.00 27.84	C
MOTA	71	C	HIS	Α	10	73.107	65.471,	25.593	1.00 28.16	C
MOTA	72	0 .	HIS	A	10	72.470	64.524	26.066	1.00 27.35	0
ATOM	73	CB	HIS		10	74.610	66.693	27.142	1.00 29.04	C
MOTA	74	CG	HIS		10	74.871	67.865	28.034	1.00 30.87	C
MOTA	75		HIS		10	75.329	69.075	27.560	1.00 30.98	N
MOTA	76		HIS		10	74.695	68.025	29.368	1.00 31.03	C
MOTA	77		HIS		10	75.423	69.931	28.563	1.00 30.39	C
MOTA	78		HIS		10	75.045	69.318	29.670	1.00 31.86	N
MOTA	79	N	THR		11	73.690	65.440	24.393	1.00 28.34	N C
ATOM	80	CA	THR		11	73.642	64.268	23.505	1.00 30.45	C
ATOM	81	C	THR		11	75.019	63.582	23.511	1.00 29.54 1.00 29.40	0
MOTA	82	.0	THR		11	75.994	64.158	23.987	1.00 29.40	C
ATOM	83	CB	THR		11	73.324	64.667	22.038 21.537	1.00 35.21	0
ATOM	84	OG1			11	74.374	65.507	21.537	1.00 33.21	C
ATOM	85.	CG2			11	72.016	65.425 62.368	22.964	1.00 32.40	N
ATOM	86	N	PHE		12	75.095 76.349	61.606	22.916	1.00 30.07	C
ATOM	87	CA C	PHE PHE		12 12	77.534	62.334	22.291	1.00 32.84	c
MOTA	88 89	0	PHE		12	78.664	62.178	22.745	1.00 32.45	0
MOTA	90	CB	PHE		12	76.155	60.280	22.167	1.00 32.22	c
MOTA	91	CG	PHE		12	75.231	59.318	22.859	1.00 32.84	. C
ATOM ATOM	92		PHE		12	75.383	59.038	24.213	1.00 32.67	C
ATOM	93		PHE		12	74.217	58.682	22.152	1.00 32.52	C
ATOM	94		PHE		12	74.535	58.137	24.854	1.00 33.67	C
ATOM	95		PHE		12	73.364	57.777	22.783	1.00 32.40	C
ATOM	96	CZ	PHE		12	73.522	57.505	24.133	1.00 32.01	C
ATOM	97	N	ASN		13	77.280	63.111	21.242	1.00 34.83	N
ATOM	98	CA	ASN		13	78.341	63.850	20.564	1.00 35.40	C
ATOM	99	C	ASN		13	79.075	64.842	21.460	1.00 34.57	C
ATOM	100	Ō	ASN		13	80.147	65.319	21.096	1.00 34.83	0
ATOM	101	СВ	ASN		13	77.783	64.602	19.349	1.00 39.42	C
MOTA	102	CG	ASN		13	77.635	63.714	18.130	1.00 44.49	. С
MOTA	103		ASN		13	78.553	62.970	17.773	1.00 47.75	0
ATOM	104		ASN			76.482	63.796	17.473	1.00 48.05	N
ATOM	105	N	GLU		14	78.501	65.153	22.621	1.00 33.44	N
MOTA	106	CA	GLU		14	79.108	66.100	23.553	1.00 33.47	C
MOTA	107	С	GLU		14	80.050	65.462	24.572	1.00 33.77	C
MOTA	108	0	GLU		14	80.608	66.157	25.418	1.00 34.50	0
ATOM	109	CB	GLU	Α	14	78.018	66.868	24.307	1.00 32.95	С

MOTA	110	CG	GLU	A	14	77.087	67.648 .	23.406	1.00	33.19		С
ATOM	111	CD	GLU	Α	14	76.050	68.434	24.175	1.00	32.32		С
ATOM	112	OE1	GLU	A	14	76.433	69.350	24.936	1.00	32.77		0
ATOM	113	OE2	GLU	A	14	74.852	68.131	24.016	1.00	31.82		0
ATOM	114	N	TYR	A	15	80.230	64.148	24.496	1.00	32.50		N
ATOM	115	CA	TYR	A	15	81.093	63.463	25.444	1.00	31.35	•	C
ATOM	116	C	TYR	Α	15	82.280	62.747	24.829	1.00	32.01		С
ATOM	117	0	TYR	-A	15	82.283	62.403	23.649	1.00	32.05		0
MOTA	118	CB	TYR	Α	15	80.286	62.435	26.236	1.00	30.88		С
MOTA	119	CG	TYR	Α	15	79.251	63.028	27.153	1.00	31.45		C
MOTA	120	CD1	TYR	A	15	79.571	63.380	28,462	1.00	31.97		C
ATOM	121	CD2	TYR	Α	15	77.947	63.241	26.710	1.00	31.39		C
ATOM	122	CE1	TYR	Α	15	78.614	63.928	29.314	1.00	33.72		C
ATOM	123	CE2	TYR		15	76.986	63.790	27.549	1.00	33:18		С
ATOM	124	CZ	TYR	Α	15	77.321	64.129	28.846	1.00	32.92	•	C
ATOM	125	OH	TYR	Α	1.5	76.363	64.677	29.669	1.00	36.12		0
MOTA	126	N	LEU	A	16	83.290	62.523	25.661		32.48		N
MOTA	127	CA	LEU	A	16	84.479	61.779	25.263	1.00	31.96		C
ATOM	128	С	LEU	Α	16	84.859	60.959	26.486	1.00	30.88		C
ATOM	129	0	LEU		16	84.541	61.336	27.609		29.12		0
MOTA	130	CB .	LEU	Α	16	85.641	62.711	24.888	1.00	31.45		C
ATOM	131	CG	LEU		16	85.562	63.515	23.583		33.88		C
ATOM	132		LEU		16	86.829	64.331	23.436		34.99		C
ATOM	133		LEU		16	85.406	62.591	22.383		33.78		Ċ
ATOM	134	N	LEU		17	85.521	59.830	26.261		31.45		N
ATOM	135	CA	LEU		17	85.977	58.966	27.347		32.43		C
MOTA	136	C	LEU		17	87.454	59.276	27.617		32.04		C
ATOM	137	0	LEU		17	88.245	59.410	26.678		32.62		ō
ATOM	138	СВ	LEU		17	85.840	57.489	26.944		31.23		C
ATOM	139	CG	LEU		17	84.423	56.919	26.852		32.03		C
ATOM	140		LEU		17	84.389	55.730	25.898		30.72		C
ATOM	141	CD2			17	83.943	56.532	28.243		29.59		C
ATOM	142	N	ILE		18	87.809	59.410	28.893		31.01		N
ATOM	143	CA	ILE		18	89.190	59.664	29.287	1.00	30.55		C
ATOM	144	C	ILE		18	89.743	58.306	29.717		30.47		C
ATOM	145	ō	ILE		18	89.188	57.659	30.598		30.46		ō
ATOM	146	СВ	ILE		18	89.273	60.651	30.471		30.96		Ċ
ATOM	147	CG1			18	88.794	62.035	30.026		31.21		C
ATOM	148	CG2	ILE		18	90.712	60.731	30.989		29.69		C
ATOM	149		ILE		18	88.792	63.066	31.139		32.55		C
ATOM	150	N	PRO		19	90.842	57.857	29.095		30.24		N
ATOM	151	CA	PRO		19	91.439	56.562	29.428		32.18		C
ATOM	152	C	PRO		19	91.766	56.336	30.903		31.60		C
MOTA	153	Õ	PRO		19	91.999	57.282	31.662		31.91		0
ATOM	154	CB	PRO		19	92.697	56.517	28.552		31.40		C
ATOM	155	CG	PRO		19	92.326	57.403	27.384		31.65		C
ATOM	156	CD	PRO		19	91.634	58.550	28.065		30.73		C
ATOM	157	N	GLY		20	91.757	55.062	31.285		31.52		N
ATOM	158	CA	GLY		20	92.092	54.655	32.638		31.25		C
ATOM	159	C	GLY			93.307	53.755	32.485		31.86		C
MOTA	160	0	GLY		20	93.903	53.696	31.403		30.12		o
ATOM	161	N	LEU		21	93.677	53.040	33.539		32.96		N
ATOM	162	CA	LEU		21	94.840	52.163	33.458		34.19		C
MOTA	163	CA	LEU		21	94.525	50.904	32.669		33.97		C
MOTA	164	0	LEU		21	93.619	50.151	33.020		34.45		0
MOTA	165	CB	LEU		21	95.330	51.770	34.863		34.43		C
ATOM	166	CG	LEU		21	96.489	50.759	34.863		34.37		C
-17 01.1	100	CG	1110	~~		JU.403	20.722	J=+90#	1.00	J=, ZU		_

MOTA	167	CD1	LEU	Α	21	97.700	51.336	34.182	1.00 30	.55		С
MOTA	168	CD2	LEU	Α	21	96.838	50.420	36.355	1.00 34	.84		С
MOTA	169	N	SER	A	22	95.269	50.688	31.592	1.00 34	1.75		N
ATOM	170	CA	SER	A	22	95.079	49.502	30.774	1.00 36	5.74		С
ATOM	171	C	SER	A	22	96.083	48.451	31.233	1.00 38	3.35		С
ATOM	172	0	SER	Α	22	97.294	48.668	31.165	1.00 36	5.70		0
ATOM	173	CB	SER	Α	22	95.313	49.827	29.300	1.00 36	5.32		С
MOTA	174	OG	SER	Α	22	94.402	50.807	28.845	1.00 37	7.15		0
MOTA	175	N	THR	Α	23	95.575	47.318	31.706	1.00 40	0.20		N
ATOM	176	CA	THR	А	23	96.429	46.235	32.183	1.00 42	2.51		С
ATOM	177	C	THR	A	23	96.838	45.318	31.036	-1.00 43	3.43		С
ATOM	178	0	THR	Α	23	96.204	45.321	29.980	1.00 44	1.38		0
ATOM	179	CB	THR	A`	23	95.711	45.414	33.258	1.00 42	2.79		С
MOTA	180	OG1	THR	Α	23	94.456	44.957	32.744	1.00 45	5.13		0
ATOM	181	CG2	THR	А	23	95.461	46.263	34.492	1.00 43	3.22		С
ATOM	182	N	VAL	A	24	97.897	44.535	31.241	1.00 43	3.96		N
ATOM	183	CA	VAL	A	24	98.383	43.632	30.198	1.00 45	5.09		С
ATOM	184	C	VAL	Α	24	97.369	42.587	29.737	1.00 45	5.87		С
ATOM	185	0	VAL	A	24	97.391	42.175	28.576	1.00 49	5.20		0
ATOM	186	CB	VAL	Α	24	99.678	42.894	30.632	1.00 45	5.95 .		C
ATOM	187	CG1	VAL	A	24	100.823	43.893	30.783	1.00 45	5.49		С
MOTA	188	CG2	VAL	Α	24	99.442	42.134	31.933	1.00 45	5.36		С
ATOM	189	N	ASP	Α	25	96.479	42.159	30.628	1.00 47	7.13		N
MOTA	190	CA	ASP	A	25	95.489	41.159	30.244	1.00 50	0.41		С
MOTA	191	C	ASP	Α	25	94.326	41.710	29.421	1.00 50	0.20		С
ATOM	192	0	ASP		25	93.519	40.940	28.909	1.00 50	0.81		0
MOTA	193	CB	ASP		25	94.936	40.430	31.479	1.00 52	2.89		С
ATOM	194	CG	ASP		25	94.232	41.361	32.446	1.00 56	5.19		С
ATOM	195	OD1	ASP	Α	25	93.566	40.864	33.381	1.00 58			0
MOTA	196		ASP		25	94.345	42.590	32.281	1.00 59			0
ATOM	197	N	CYS	А	26	94.234	43.030	29.270	1.00 49	9.99		N
ATOM	198	CA	CYS	A	26	93.124	43.581	28.497	1.00 48	3.97		С
ATOM	199	G.	CYS		26	93.408	43.743	27.018	1.00 49	9.15		С
ATOM	200	0	CYS	Α	26	93.939	44.764	26.581	1.00 48	3.97		0
MOTA	201	CB	CYS		26	92.660	44.937	29.047	1.00 47	7.43		С
ATOM	202	SG	CYS	Α	26	90.937	45.377	28.585	1.00 43	3.74		s
ATOM	203	N	ILE	А	27	93.054	42.722	26.250	1.00 49	9.92		N
MOTA	204	CA	ILE	Α	27	93.204	42.774	24.810	1.00 50	0.73		С
ATOM	205	C	ILE	Α	27	91.781	42.593	24.300	1.00 50	0.66		C
MOTA	206	0	ILE	Α	27	90.960	41.941	24.953	1.00 50	0.24		0
MOTA	207	CB	ILE	Α	27	94.111	41.644	24.271	1.00 52	2.78		Ç
ATOM	208	CG1	ILE	Α	27	93.547	40.280	24.661	1.00 53	3.35		С
MOTA	209	CG2	ILE	A	27	95.530	41.814	24.810	1.00 52	2.47		С
MOTA	210	CD1	ILE	Α	27	94.339	39.120	24.094	1.00 56	5.96		С
MOTA	211	N	PRO	Α	28	91.460	43.188	23.145	1.00 50	0.63		N
ATOM -	212	CA	PRO	Α	28	90.126	43.096	22.548	1.00 50	0.44		С
ATOM	213	C	PRO	A	28	89.496	41.705	22.535	1.00 50	71		C
ATOM	214	0	PRO	А	28	88.329	41.545	22.895	1.00 50	08.0		0
MOTA	215	CB	PRO	A	28	90.349	43.653	21.148	1.00 50	0.84		С
MOTA	216	CG	PRO	A	28	91.336	44.746	21.407	1.00 50	0.51		С
MOTA	217	CD	PRO	A	28	92.325	44.085	22.356	1.00 50	0.67		С
MOTA	218	N	SER	Α	29	90.265	40.700	22.131	1.00 50	0.62		N
ATOM	219	CA	SER	A	29	89.745	39.340	22.060	1.00 49	9.43		С
ATOM	220	C	SER		29	89.327	38.758	23.409	1.00 48	3.35		C
ATOM	221	0	SER	Α	29	88.575	37.786	23.456	1.00 49	9.06		0
ATOM	222	CB	SER	Α	29	90.767	38.416	21.383	1.00 51			С
ATOM	223	OG	SER	A	29	91.969	38.322	22.126	1.00 53	3.31		0

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MOTA	224	N	ASN		30	89.801	39.335	24.508		45.87		N
ATOM `	225	CA	ASN		30	89.414	38.824	25.819		44.49		С
ATOM	226	C	ASN	Α	30	88.238	39.593	26.433	1.00	42.49		С
MOTA	227	0	ASN	Α	30	87.765	39.248	27`.518	1.00	42.16		0
MOTA	228	CB	ASN	Α	30	90.594	38.854	26.793	1.00	46.85		С
ATOM	229	CG	ASN	Α	30	91.698	37.892	26.404	1.00	50.18		С
ATOM	230		ASN		30	91.443	36.831	25.828		52.17		ō
		ND2										
ATOM	231				30	92.936	38.250	26.734		51.10		N
MOTA	232	N	VAL		31	87.768	40.632	25.746		38.75		N
ATOM	233	CA	LAV	Α	31	86.651	41.422	26.258	1.00	36.68		С
MOTA	234	C	VAL	А	31	85.333	40.660	26.097	1.00	35.73		С
MOTA	235	0	VAL	Α	31	85.033	40.127	25.034	1.00	33.64		0
MOTA	236	CB	VAL		31	86.558	42.802	25.538		36.09		С
ATOM	237		VAL		31	85.357	43.593	26.053		34.31		Ċ
ATOM	238		VAL		31	87.839	43.598	25.782		35.58		C
ATOM	239	N	ASN		32	84.564	40.589	27.174		35.18	•	N
MOTA	240	CA	ASN		32		.39.894	27.152		35.95		Ċ
ATOM	241	С	ASN		32	82.173	40.938	27.055	1.00	35.44		Ċ
ATOM	242	0	ASN	Α	32	82.050	41.802	27.918	1.00	36.50		0
ATOM	243	CB	ASN	Α	32	83.150	39.041	28.423	1.00	36.77		С
MOTA	244	CG	ASN	Α	32	81.740	38.509	28.644	1.00	38.35		C
ATOM	245		ASN		32	80.908	38.499	27.739		37.24		Ō
ATOM	246		ASN		32	81.475	38.050	29.863		40.73		N
ATOM	247	N	LEU		33	81.373	40.863	25.995		34.92		N
MOTA	248	CA	LEU		33	80.291	41.822	25.799		34.68		С
ATOM	249	C	LEU	A	33	78.908	41.292	26.161	1.00	34.77		С
ATOM	250	0	LEU	А	33	77.900	41.799	25.663	1.00	35.47		0
ATOM	251	CB	LEU	A	33	80.282	42.329	24.348	1.00	34.75		С
ATOM	252	CG	LEU	Α	33	81.474	43.173	23.894	1.00	35.98		С
ATOM	253	CD1			33	81.283	43.601	22.451		35.27		С
ATOM	254		LEU		33	81.621	44.392	24.799		35.37		Ċ
ATOM	255	N	SER		34	78.851	40.275	27.016		33.98		N
ATOM	256	CA	SER		34	77.566	39.724	27.449		34.88		C
ATOM	257	C	SER		34	76.841	40.762	28.301		34.25		C
ATOM	258	0	SER		34	77.472	41.554	28.998	1.00	33.82	•	0
ATOM	259	CB	SER	Α	34	77:770	38.456	28.284	1.00	35.12		С
ATOM	260	OG	SER	A	34	78.323	37.420	27.491	1.00	42.00		0
ATOM	261	N	THR	Α	35	75.516	40.748	28.263	1.00	32.80		N
ATOM	262	CA	THR	Α	35	74.754	41.708	29.034		31.26		С
ATOM	263	C :	THR		35	73.342	41.170	29.282		31.11		C
ATOM	264	Õ	THR		35	72.798	40.424	28.466		31.76		Ö
ATOM								28.280				
	265	CB	THR		35	74.706	43.068			31.41		C
ATOM	266	OG1			35	74.416	44.123	29.202		30.49		0
ATOM	267	CG2			35	73.644	43.043	27.184		30.33		С
ATOM	268	N	PRO		36	72.736	41.530	30.422	1.00	29.74		И
ATOM	269	CA	PRO	Α	36	71.385	41.070	30.758	1.00	30.21		С
ATOM	270	C	PRO	А	36	70.264	41.741	29.958	1.00	31.22		С
ATOM	271	0	PRO	Α	36	70.291	42.953	29.713	1.00	31.11		0
ATOM	272	CB	PRO	,	36	71.284	41.366	32.253		30.05		С
ATOM	273	CG	PRO		36	72.114	42.613	32.397		27.96		Ċ
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ATOM	274	CD	PRO		36	73.322	42.310	31.529		28.83		
ATOM	275	N	LEU		37	69.276	40.943	29.566		30.99		N
ATOM	276	CA	LEU		37	68.142	41.438	28.805		31.62		С
MOTA	277	C	LEU		37	66.910	41.656	29.683	1.00	32.81		С
ATOM	278	0	LEU	А	37	66.165	42.618	29.485	1.00	34.25		0
ATOM	279	CB	LEU	Α	37	67.788	40.459	27.681	1.00	31.89		C
ATOM	280	CG	LEU		37	66.642	40.913	26.764		32.36		С
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MOTA	281	CD1	LEU	Α	37	67.124	42.073	25.888	1.00	31.95		С
ATOM	282	CD2	LEU	Α	37	66.175	39.757	25.892	1.00	31.83		С
ATOM	283	N	VAL	А	38	66.691	40.774	30.655	1.00	32.12		N
MOTA	284	CA	VAL	Α	38	65.521	40.901	31.517	1.00	31.54		С
ATOM	285	C	VAL	Α	38	65.869	40.922	33.004	1.00	32.49	-	С
MOTA	286	0	VAL	Α	38	66.867	40.344	33.427	1.00	33.79		0
ATOM	287	CB	VAL	Α	38 .	64.486	39.772	31.219	1.00	31.66		c ·
ATOM	288	CG1	VAL	Α	38	64.026	39.872	29.765	1.00	28.94	•	С
ATOM	289	CG2	VAL	Α	38	65.093	38.398	31.482	1.00	29.49		С
ATOM	290	N	LYS	А	39	65.025	41.584	33.789	1.00	31.86		N
ATOM	291	CA	LYS		39	65.246	41.742	35.219	1.00	33.55		С
ATOM	292	С	LYS		39	65.423	40.464	36.025		34.23		Ċ
ATOM	293	0	LYS		39	64.893	39.415	35.678		34.30		0
ATOM	294	СВ	LYS		39	64.112	42.560	35.842		34.12		C
ATOM	295	CG	LYS		39	62.743	41.886	35.791		34.26		Ċ
ATOM	296		LYS		39	61.727	42.681	36.588		34.93		C
ATOM	297	CE	LYS		39	60.368	41.981	36.614		35.16		c
ATOM	298	NZ	LYS		39	59.412	42.684	37.515		34.58		N
ATOM	299		PHE		40	66.175	40.592	37.114		34.89		N
ATOM	300	CA	PHE		40	66.454	39.499	38.032		36.02		C
ATOM	301	C	PHE		40	66.698	40.089	39.416		37.46		C
ATOM	302	ō	PHE		40	66.849	41.303	39.562		38.06		0
ATOM	303	СВ	PHE		40	67.687	38.699	37.582		34.23		C
ATOM	304	CG	PHE		40	68.926	39.535	37.376		33.77		C
ATOM	305		PHE		40	69.178	40.142	36.145		32.47		C
ATOM	306		PHE		40	69.844	39.704	38.405		31.36		C
ATOM	307		PHE		40	70.326	40.899	35.945		31.93		C
ATOM	308	CE2	PHE		40	70.320	40.460	38.218		31.43		C
ATOM	309	CZ	PHE		40	70.998	41.060	36.216		31.40		C
ATOM	310	N .	GLN		41	66.728	39.227	40.427		38.80		
ATOM	311	CA			41							N C
ATOM	312	CA	GLN GLN		41	66.954	39.653	41.800		40.40		C
ATOM		0				68.439	39.656	42.110			•	
ATOM	313 314	CB	GLN GLN		41 41	69.238	39.044	41.402		39.75		0
ATOM						66.256	38.705	42.790		44.12		C
ATOM	315 316	CG CD	GLN		41	64.735	38.752	42.795		49.04		C
			GLN GLN		41	64.188	40.059	43.352		51.98		C
MOTA	317	OE1 NE2			41	64.464	40.433	44.501		54.77		0
ATOM ATOM	318		GLN		41	63.406	40.761	42.541		52.25		N
	319	N	LYS		42	68.798	40.353	43.179		39.91		N
ATOM	320	CA	LYS		42	70.178	40.423	43.627		41.35		C
MOTA	321	C	LYS		42	70.701	38.997	43.872		41.68		C
ATOM	322	0	LYS		42	69.993	38.157	44.428		40.20		0
ATOM	323	CB	LYS		42	70.236	41.226	44.921		42.49		C
ATOM	324	CG	LYS		42	71.606	41.323	45.551		45.67		C
ATOM	325	CD	LYS		42	71.501	42.014	46.902		47.42		C
ATOM	326	CE	LYS		42	72.844	42.067	47.605		48.87		С
ATOM	327	NZ	LYS		42	72.721	42.779	48.906		52.09		N
ATOM	328	N	GLY		.43	71.929	38.728	43.442		41.55		N
ATOM	329	CA	GLY		43	72.511	37.412	43.644		40.73		C
ATOM	330	C	GLY		43	72.226	36.425	42.532		40.52		C
ATOM	331	0	GLY		43	72.807	35.341	42.496		40.95		0
ATOM	332	N	GLN		44	71.330	36.788	41.625		40.46		N
ATOM	333	CA	GLN		44	70.992	35.912	40.511		41.27		C
ATOM	334	C	GLN		44	71.591	36.440	39.211		41.60		C
ATOM	335	0	GLN		44	72.292	37.450	39.196		40.78		0
ATOM	336	CB	GLN		44	69.471	35.822	40.342		42.42		C
ATOM	337	CG	GLN	Α	44	68.688	35.691	41.637	1.00	45.60		C

ATOM	338	CD	GLN	Α	44	67.186	35.582	41.402	1.00 47.33		· C
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MOTA	339	OE1	GLN		44	66.621	36.293	40.565	1.00 48.58		0
MOTA	340	NE2	GLN	Α	44	66.533	34.703	42.149	1.00 46.68		N
MOTA	341	N	GLN	A	45	71.308	35.726	38.127	1.00 42.62		N
MOTA	342	CA	GLN	А	45	71.741	36.089	36.784	1.00 43.67		C
MOTA	. 343	C	GLN	Α	45	70.443	36.216	35.999	1.00 41.83		C
MOTA	344	0	GLN	Α	45	69.439	35.611	36.367	1.00 40.98		0
ATOM	345	CB	GLN	Α	45	72.593	34.981	36.153	1.00 46.80		С
MOTA	346	CG	GLN	Α	45	73.929	34.741	36.833	1.00 52.13		C
MOTA	347	CD	GLN	Α	45	74.909	35.872	36.601	1.00 54.67		C
ATOM	348	OE1	GLN	Α	45	75.420	36.047	35.489	1.00 57.71		0
MOTA	349	NE2	GLN	Α	45	75.175	36.653	37.647	1.00 54.39		N
ATOM	350	N	SER	Α	46	70.458	36.999	34.928	1.00 39.93		N
ATOM	351	CA	SER	Α	46	69.268	37.162	34.110	1.00 38.73		C
ATOM	352	C	SER	Α	46	69.005	35.868	33.347	1.00 39.01		C
MOTA	353	0	SER	Α	46	69.942	35.211	32.906	1.00 39.13		0
MOTA	354	CB	SER	Α	46	69.464	38.304	33.113	1.00 36.60		C
ATOM	355	OG	SER	Α	46	68.330	38.437	.32.280	1.00 35.88		0
MOTA	356	N	GLU	Α	47	67.733	35.511	33.190	1.00 39.22		N
ATOM	357	CA	GLU	A	47	67.363	34.297	32.463	1.00 39.59		C
MOTA	358	C	GLU	A	47	67.762	34.400	31.000	1.00 38.86		C
ATOM	359	0	$\mathtt{GLU}$	Α	47	67.904	33.385	30.316	1.00 38.01	•	0
MOTA	360	CB	GLU	Α	47	65.857	34.057	32.563	1.00 41.44		C
MOTA	361	CG	$\operatorname{GLU}$	A	47	65.365	33.806	33.978	1.00 44.53		C
MOTA	362 ·	CD	GLU	Α	47	63.853	33.843	34.073	1.00 47.63		C
MOTA	363	OE1	GLU	Α	47	63.197	32.987	33.436	1.00 49.95		0
MOTA	364	OE2	GLU	Α	47	63.321	34.732	34.777	1.00 49.50		0
MOTA	365	N	ILE		48	67.920	35.631	30.514	1.00 37.02		N
MOTA	366	CA	ILE	Α	48	68.318	35.856	29.126	1.00 35.30		C
MOTA	367	C	ILE		48	69.474	36.854	29.055	1.00 34.82		C _.
MOTA	368	0	ILE		48	69.372	37.982	29.538	1.00 34.21		0
MOTA	369	CB	ILE		48	67.144	36.400	28.273	1.00 35.95		C
MOTA	370	CG1			48	65.958		28.328	1.00 37.12		C
MOTA	371	CG2			48	67.595	36.583	26.836	1.00 34.56		C
ATOM	372	CD1			48	64.768	35.879	27.509	1.00 37.86		C.
MOTA	373	N	ASN		49	70.579	36.426	28.462	1.00 34.10		N
ATOM .	374	CA	ASN		49	71.739	37.285	28.323	1.00 34.92		C
MOTA	375	C	ASŅ		49	72.160	37.365	26.866	1.00 35.76		C O
MOTA	376	0	ASN		49	72.383	36.341	26.218	1.00 36.32		C
MOTA	377	CB	ASN		49	72.903		29.169	1.00 35.35		C
MOTA	378	CG	ASN		49	72.634	36.856	30.660	1.00 37.43		0
ATOM	3 <b>7</b> 9		ASN		49	72.802	37.917	31.263	1.00 34.90 1.00 36.59		N
MOTA	380		ASN		49	72.193	35.755				N
MOTA	381	N	LEU		50	72.242	38.582	26.342	1.00 34.27		C
MOTA	382	CA	LEU		50	72.682	38.770		1.00 33.47		C
MOTA	383	C	LEU		50	74.184		24.991	1.00 33.03 1.00 31.70		0
MOTA	384	0	LEU		50	74.809		26.040	1.00 31.70		C
MOTA	385	CB	LEU		50	72.444	40.213	24.522 24.715	1.00 33.23		C
MOTA	386	CG	LEU		50	71.041	40.784 42.270	24.713	1.00 33.73		C
MOTA	387		LEU		50	71.050		23.846	1.00 35.37		C
ATOM	388		LEU		50 51	70.054		23.855	1.00 33.13		N
MOTA	389	N	LYS		51	74.766		23.815	1.00 33.54		C
MOTA	390	CA	LYS		51 51	76.208		23.335	1.00 33.00		C
ATOM	391	C	LYS		51 51	76.902		23.532	1.00 32.33		0
MOTA	392	O	LYS		51 51	78. <b>1</b> 09		22.946	1.00 32.77		C
MOTA	393	CB	LYS		51 51	76.531 75.984		23.593	1.00 34.02		C
MOTA	394	CG	LYS	A	51	15.904	JJ. <del>4</del> 00	25.555	1.00 57.45		_

ATOM	395	CD	LYS	Α	51	76.413	34.136	22.897	1.00 39.84		C
ATOM	396	CE	LYS	Α	51	75.893	32.920	23.663	1.00 40.88		С
MOTA	397	NZ	LYS	Α	51	76.295	31.643	22.997	1.00 43.33		N
ATOM	398	N	ILE	Α	52	76.119	40.054	22.708	1.00 31.66		N
ATOM	399	CA	ILE		52	76.585	41.370	22.274	1.00 31.00		С
ATOM	400	C	ILE		52 .	75.425	42.297	22.651	1.00 31.49		С
	401	0	ILE		52	74.257	41.937	22.498	1.00 31.89		0
ATOM						76.912	41.454	20.750	1.00 31.40		Ċ
ATOM	402	CB	ILE		52						C
ATOM	403		ILE		52	75.685	41.121	19.892	1.00 31.59		
ATOM	404	CG2	ILE		52	78.089	40.538	20.432	1.00 31.15		C
ATOM	405	CD1			52	75.900	41.415	18.400	1.00 29.50		C
ATOM	406	N	PRO	Α	53	75.733	43.499	23.154	1.00 31.49		N
MOTA	407	CA	PRO	Α	53	74.731	44.482	23.579	1.00 31.87		C
ATOM	408	C	PRO	Α	53	73.958	45.252	22.506	1.00 32.48		C
MOTA	409	0	PRO	Α	53	73.645	46.428	22.698	1.00 33.45		0
MOTA	410	CB	PRO	Α	53	75.544	45.412	24.468	1.00 31.07		C
ATOM	411	CG	PRO		53	76.853	45.479	23.713	1.00 31.12		C
ATOM	412	CD	PRO		53	77.101	44.034	23.325	1.00 30.40		C
ATOM	413	N	LEU		54	73.630	44.602	21.395	1.00 31.62		N
	414	CA	LEU		54	72.901	45.279	20.331	1.00 30.89		C
ATOM							44.592	19.986	1.00 31.85		C
ATOM .	415	C	LEU		54	71.582			1.00 31.83		0
MOTA	416	0 .	LEU		54	71.524	43.365	19.872			c
ATOM	417	CB	LEU		54	73.767	45.347	19.069	1.00 29.66		
ATOM	418	CG	LEU		54	75.192	45.900	19.182	1.00 30.68		C
ATOM	419		LEU		54	75.876	45.810	17.824	1.00 29.65		C
MOTA	420	CD2	LEU	Α	54	75.162	47.347	19.678	1.00 30.19		C
MOTA	421	N	VAL	Α	55	70.519	45.377	19.840	1.00 31.15		N
ATOM	422	CA	VAL	A	55	69.230	44.830	19.441	1.00 30.86		C
ATOM	423	C	VAL	Α	55	68.692	45.737	18.333	1.00 32.57		C
MOTA	424	0	VAL		55	68.876	46.956	18.385	1.00 33.70		0
MOTA	425	СВ	VAL		55	68.214	44.757	20.618	1.00 29.59		С
ATOM	426		VAL		55	68.833	44.009	21.786	1.00 28.25		C
ATOM	427		VAL		55	67.750	46.146	21.025	1.00 29.12		C
ATOM	428	N	SER		56	68.058	45.144	17.322	1.00 32.00		N
			SER		56	67.511	45.914	16.207	1.00 31.93		C
ATOM	429	CA					46.469		1.00 31.63		Ċ
ATOM	430	C	SER		56	66.134		16.556	1.00 31.03		.0
ATOM	431	0	SER		56	65.324	45.812	17.214			
ATOM	432	CB	SER		56	67.459	45.056	14.929	1.00 31.63		C
ATOM	433	OG	SER		56	66.668	43.895	15.102	1.00 31.84		0
MOTA	434	N	ALA	Α	57	65.891	47.697	16.115	1.00 31.38		N
ATOM	435	CA	ALA	А	57	64.654	48.419	16.395	100 31.55		C
MOTA	436	C	ALA	A	57	63.361	47.756	15.907	1.00 32.70		C
MOTA	437	0	ALA	Α	57	63.351	47.012	14.922	1.00 33.02		0
ATOM	438	CB	ALA	Α	57	64.764	49.833	15.836	1.00 29.58		C
ATOM	439	N	ILE	Α	58	62.277	48.047	16.620	1.00 32.44		. N
ATOM	440	CA	ILE		58	60.950	47.511	16.328	1.00 33.86		C
ATOM	441	C	ILE		58	60.380	48.325	15.173	1.00 34.14		C
ATOM	442	Ö	ILE		58	59.463	49.129	15.359	1.00 34.72		0
ATOM	443	CB	ILE		58	60.032	47.654	17.578	1.00 32.65		C
	444		ILE		58	60.827	47.277	18.835	1.00 33.43		C
ATOM											C
ATOM	445		ILE		58	58.800	46.759	17.444	1.00 30.11		
ATOM `	446		ILE		58	60.068	47.428	20.135	1.00 31.89		C
ATOM	447	N.	MET		59	60.931	48.111	13.982	1.00 34.79		N
ATOM	448	CA	MET		59	60.523	48.870	12.803	1.00 35.21		C
MOTA	449	C	MET		59	60.363	48.024	11.545	1.00 36.00	•	C
MOTA	450	0	MET	Α	59	61.151	47.107	11.287	1.00 34.61		0
MOTA	451	CB	MET	Α	59	61.554	49.971	12.525	1.00 35.03		С

MOTA	452	CG	MET	A	59	61.851	50.887	13.706	1.00	34.37			С
ATOM	453	SD	MET	A	59	63.181	52.051	13.323	1.00	35.17			S
MOTA	454	CE	MET	A	59	62.401	53.057	12.081	1.00	35.07			С
MOTA	455	N	GLN	A	60	59.353	48.366	10.748	1.00	37.49			N
MOTA	456	CA	GLN	A	60	59.063	47.649	9.509	1.00	39.05			С
MOTA	457	С	GLN	Α	60	60.275	47.600	8.594	1.00	38.95			С
ATOM	458	0	GLN	A	60	60.506	46.603	7.915	1.00	39.70			0
ATOM	459	CB	GLN		60	57.927	48.329	8.738	1.00	39.93			С
MOTA	460	CG	GLN		60	56.671	48.629	9.532	1.00	41.07			С
ATOM	461	CD	GLN		60	55.609	49.290	8.665	1.00	42.66			С
ATOM	462	OE1	GLN		60	55.930	50.010	7.717		42.94			0
ATOM	463	NE2	GLN		60	54.342	49.058	8.992		42.62			N
ATOM	464	N	SER		61	61.046	48.683	8.578		39.09			N
ATOM	465	CA	SER		61	62.215	48.770	7.705		38.98			С
ATOM	466	C.	SER		61	63.506	48.217	8.296		38.63			C
ATOM	467	0	SER		61	64.577	48.352	7.694		38.93			0
ATOM	468	СВ	SER		61	62.436	50.228	7.280		39.27			C
ATOM	469	OG	SER		61	62.568	51.078	8.409		42.11			0
	470					63.407	47.578	9.457		37.45			N
ATOM		N	VAL		62		47.048	10.112		36.30			C
ATOM	471	CA	VAL		62	64.593	47.040			37.04			C
ATOM	472	C	VAL		62	64.535		10.536					
ATOM	473	0	VAL		62	65.304	44.765	10.050		38.38			0
ATOM	474	CB	VAL		62	64.939	47.869	11.382		36.10			C
ATOM	475		VAL		62	66.168	47.274	12.069		34.59			C
ATOM	476	CG2	VAL		62	65.175	49.330	11.016		35.17			C
ATOM	477	N	SER		63	63.621	45.275	11.444		37.88			N
MOTA	478	CA	SER		63	63.540	43.929	11.982		38.55			C
ATOM	479	C	SER		63	62.557	42.938	11.368		39.50			С
ATOM	480	0	SER		63	61.454	42.727	11.879		37.63			0
ATOM	481	CB	SER		63	63.319	44.013	13.495		38.61			С
ATOM	482	OG	SER	А	63	64.401	44.694	14.120		36.71			0
ATOM	483	N ·	GLY	Α	64	62.991	42.329	10.268	1.00	39.83			N
ATOM	484	CA	$\mathtt{GLY}$	Α	64	62.201	41.317	9.597	1.00	41.35			С
MOTA	485	C	GLY	А	64	62.814	39.992	10.023	1.00	43.17			С
ATOM	486	0	GLY	Α	64	63.710	39.973	10.874	1.00	39.88	•		0
ATOM	487	N	GLU	Α	65	62.373	38.884	9.432	1.00	44.98			N
ATOM	488	CA	GLU	Α	65	62.913	37.593	9.832	1.00	47.09			С
MOTA	489	C	GLU	A	65	64.384	37.401	9.484	1.00	45.97			С
ATOM	490	0	GLU	Α	65	65.129	36.825	10.274	1.00	45.63			0
ATOM	491	CB	GLU	Α	65	62.069	36.447	9.259	1.00	50.39			С
ATOM	492	CG	GLU	Α	65	62.087	36.305	7.758	1.00	56:03			С
ATOM	493	CD	GLU	A	65	61.206	35.158	7.297	1.00	60.65			С
ATOM	494	OE1	GLU	A	65	59.968	35.256	7.478	1.00	62.24			0
ATOM	495		GLU		65	61.752	34.158	6.768	1.00	61.62			0
ATOM	496	N	LYS		66	64.814	37.885	8.322	1.00	45.39			N
ATOM	497	CA.	LYS		66	66.216	37.740	7.941	1.00	45.57			С
ATOM	498	С	LYS		66	67.118	38.490	8.917	1.00	43.76			C
ATOM	499	0	LYS		66	68.197	38.014	9.275		43.26			0
ATOM	500	СВ	LYS		66	66.452	38.255	6.518		48.10			С
ATOM	501	CG	LYS		66	66.051	37.272	5.426		53.08			·C
ATOM	502	CD	LYS		66 -	66.353	37.827	4.032		56.63			C
ATOM	503	CE	LYS		66	65.933	36.847	2.937		58.88			C
ATOM	504	NZ	LYS		66	66.138	37.403	1.561		59.62		-	N
ATOM	505	N	MET		67	66.671	39.665	9.347		41.61			N
ATOM	506	CA	MET		67	67.440	40.468	10.290		40.17			C
ATOM	507	CA	MET		67	67.552	39.730	11.625		39.71			C
	508	0					39.730	12.199		38.59			0
MOTA	508	. •	MET	M	67	68.638	39.013	16.177	1.00	50.59			J

MOTA	509	СВ	MET	A	67	66	6.761	41.822	10.507		39.65		C
MOTA	510	CG	MET	A	67		7.451	42.722	11.525		38.90		С
MOTA	511	SD	MET	Α	67	69	9.110	43.219	11.014		38.59		S
MOTA	512	CE	MET	A	67	68	8.730	44.370	9.680		37.11		С
ATOM	513	N	ALA	A	68	6.0	6.422	39.217	12.102		38.12		N
ATOM	514	CA	ALA	A	68	6	6.370	38.505	13.371		38.12		C
MOTA	515	С	ALA	Α	68	6'	7.314	37.306	13.407		38.48		C
MOTA	516	0	ALA	Α	68	6	7.919	37.009	14.437		38.33		0
MOTA	517	CB	ALA	Α	68	6	4.947	38.064	13.652		37.40		C
MOTA	518	N	ILE	Α	69		7.435	36.622	12.275		38.50	•	N
MOTA	519	CA	ILE	Α	69		8.308	35.461	12.163		38.32		C
MOTA	520	C	ILE		69		9.774	35.896	12.129		37.75		C
MOTA	521	0	ILE		69		0.601	35.383	12.883		38.40		0
ATOM	522	CB	ILE		69		7.981	34.656	10.874		40.02		C
ATOM	523	CG1	ILE		69		6.603	33.998	11.006		40.60		C
MOTA	524	CG2	ILE		69.		9.042	33.599	10.625		38.98		C
ATOM	525	CD1	ILE		69		6.013	33.545	9.678		41.31		C
MOTA	526	N	ALA		70		0.084	36.847	11.254		37.08		N
MOTA	527		ALA		70		1.442	37.348	11.109		36.18		C
MOTA	528.	С	ALA.		70		2.000	37.959	12.392		36.22		0
MOTA	529	0	ALA		70		3.182	37.796	12.695		36.51		C
MOTA	530	CB	ALA		70		1.499	38.366	9.987		36.62		N
MOTA	531	N	LEU		71		1.155	38.661	13.142		35.64		C
MOTA	532	CA	LEU		71		1.593	39.293	14.381		35.41		C
MOTA	533	C	LEU		71		1.752	38.281	15.511		35.81		0
ATOM	534	0	LEU		71		2.707	38.353	16.282		34.47 33.24		C
MOTA	535	CB	LEU		71		0.617	40.400	14.792 16.061		33.66		C
ATOM	536	CG	LEU		71		0.921	41.215	16.110		31.27		C
ATOM	537		LEU		71		2.391	41.629 42.451	16.110		31.14		C
ATOM	538		LEU		71		0.021	37.337	15.608		37.05		N
ATOM	539	N	ALA		72		0.822	36.317	16.648		38.69		C
MOTA	540	CA	ALA		72		0.906 2.166	35.476	16.445		40.01		C
ATOM	541	C	ALA		72		2.166	34.988	17.411		39.86		o
MOTA	542	O	ALA		72 72		9.665	35.422	16.620		37.80		C
MOTA	543	CB	ALA		73		2.570	35.304	15.188		40.95		N
MOTA	544	N	ARG ARG		73 73		3.761	34.525	14.874		43.10		C
MOTA	545	CA C	ARG		73 ·		5.701	35.169	15.464		43.29		C
MOTA	546 547	0	ARG		73 ·		5.963	34.477	15.807		42.95		Ö
ATOM		CB	ARG		73		3.940	34.384	13.359		45.58		C
ATOM ATOM	548 549	CG	ARG		73		3.014	33.367	12.707		49.18		C
ATOM	550	CD	ARG		73		3.285	33.246	11.210		52.08		С
ATOM	551	NE	ARG		73		72.430	32.238	10.591		55.80		N
ATOM	552	CZ	ARG		73		72.264	32.093	9.278		58.09		Ç
ATOM	553		ARG		73		72.897	32.895	8.427		58.20		N
ATOM	554		ARG		73		71.460	31.144	8.813	1.00	58.98		N
ATOM	555	N	GLU		74		74.976	36.495	15.585		42.49		N
ATOM	556	CA	GLU		74		76.103	37.239	16.129	1.00	41.53		С
ATOM	557	C	GLU		74		75.987	37.478	17.631		39.63		С
ATOM	558	Ō	GLU		74		76.896	38.031	18.242	1.00	40.05		0
MOTA	559	CB	GLU		74		76.255	38.577	15.401	1.00	42.87		C
ATOM	560	CG	GLU		74		76.467	38.458	13.892	1.00	45.91		С
ATOM	561	CD	GLU		74		77.673	37.595	13.522	1.00	49.55		С
ATOM	562		GLU		74		78.768	37.813	14.094	1.00	50.07		0
ATOM	563		GLU		74		77.524	36.704	12.653	1.00	50.61		0
ATOM	564	N	GLY		75		74.869	37.074	18.229	1.00	38.37		N
ATOM	565	CA	GLY		75		74.716	37.250	19.664	1.00	38.10		С

		_		_		72 715	20 207	20 122	1 00	20 20		C
MOTA	566	С	GLY		75	73.715	38.287	20.132	1.00			C
ATOM	567	0	GLY		75	73.517	38.458	21.337	1.00			0
MOTA	568	N	GLY	A	76	73.092	38.987	19.192		37.09		N
MOTA	569	CA	GLY		76	72.107	39.990	19.549		36.51		С
ATOM	570	C	GLY	Α	76	70.708	39.449	19.312		36.82		C
ATOM	571	0	GLY	A	76	70.546	38.266	18.989	1.00	36.23		0
MOTA	572	N	ILE	A	77	69.698	40.298	19.477	1.00	35.24		N
MOTA	573	CA	ILE	Α	77	68.316	39.875	19.259	1.00	34.74		С
ATOM	574	С	ILE	Α	77	67.536	40.962	18.518	1.00	35.14		C
ATOM	575	0	ILE	Α	77	67.837	42.159	18.634	1.00	34.83		0
ATOM	576	СВ	ILE		77	67.609	39.552	20.602	1.00	33.95		С
ATOM	577	CG1	ILE		77	66.389	38.655	20.350	1.00	34.82		C
ATOM	578	CG2	ILE		77	67.179	40.850	21.305		33.35		С
ATOM	579		ILE		77	65.636	38.255	21.619		31.17		C
ATOM	580	N	SER		78	66.543	40.539	17.744		34.83		N
		CA	SER		78	65.711	41.467	16.993		33.97		C
MOTA	581					64.300	41.484	17.547		34.42		C
ATOM	582	C	SER		78 78		40.484	18.074		35.04		0
ATOM	583	0	SER		78	63.817						C
MOTA	584	CB	SER		78	65.645	41.068	15.513		32.74	. : -	
ATOM	585	OG	SER		78	66.870	41.295	14.848		30.88		0
ATOM	586	N	PHE		79	63.641	42.629	17.439		34.58		N
ATOM	587	CA	PHE		79	62.270	42.740	17.891		35.16		C
ATOM	588	С	PHE		79	61.405	42.906	16.646		35.89		C
ATOM	589	0	PHE		79	61.253	44.011	16.126		36.16		0
MOTA	590	CB	PHE	A	79	62.094	43.929	18.846		33.75		C
MOTA	591	CG	PHE	A	79	62.664	43.688	20.219		34.30		C
ATOM ·	592	CD1	PHE	Α	79	64.016	43.911	20.481		35.61		C
MOTA	593	CD2	PHE	Α	79	61.862	43.182	21.238	1.00	33.96		C
ATOM	594	CE1	PHE	A	79	64.559	43.626	21.745	1.00	35.47	•	С
ATOM	595	CE2	PHE	A	79	62.395	42.893	22.503	1.00	33.04		С
MOTA	596	CZ ·	PHE	A	79 ·	63.741	43.115	22.755	1.00	33.81		С
MOTA	597	N	ILE		80	60.869	41.790	16.158	1.00	35.40		N
MOTA	598	CA	ILE		80	60.011	41.791	14.977	1.00	35.16		С
ATOM	599	С	ILE		80	58.951	42.878	15.136	1.00	35.68		C
ATOM	600	0	ILE		80	58.241	42.916	16.149	1.00	35.60		0
MOTA	601	СВ	ILE		80	59.317	40.417	14.802	1.00	35.87		C
MOTA	602	CG1	ILE		80	60.373	39.319	14.621		35.71		C
ATOM	603	CG2	ILE		80	58.381	40.446	13.592		35.14		С
ATOM	604	CD1				61.235	39.494	13.386		34.65		C
ATOM	605	N	PHE		81	58.838	43.754	14.140		35.48		N
ATOM	606	CA	PHE		81	57.879	44.848	14.221		37.39		C
ATOM	607	C	PHE		81	56.427	44.423	14.437		37.98		C
MOTA	608	0	PHE		81	55.953	43.440	13.863		38.21		0
					81	57.989	45.773	12.990		38.37		C
ATOM	609	CB	PHE				45.773	11.666		39.29		C
ATOM	610	CG	PHE		81	57.733				39.25		C
ATOM	611		PHE		81	58.693	44.272	11.089		39.78		C
ATOM	612		PHE		81	56.543	45.315	10.978				
MOTA	613		PHE		81	58.476	43.681	9.838		39.50		C
ATOM	614		PHE		81	56.313	44.731	9.729		40.29		C
ATOM	615	CZ	PHE		81	57.284	43.911	9.158		39.87		C
MOTA	616	N	GLY		82	55.730	45.178	15.281		38.14		N
MOTA		CA	GLY		82	54.341	44.878	15.570		39.76		C
ATOM	618	C	GLY	Α	82	53.374	45.678	14.720		40.57		C
ATOM	619	0	GLY	Α	82		45.550	14.869		41.33		0
MOTA	620	N	SER		83	53.909	46.504	13.826		40.23		N
ATOM	621	CA	SER	Α.	83	53.076	47.313	12.945		41.14		C
ATOM	622	C	SER	A	83	52.678	46.522	11.698	1.00	41.79		С

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ATOM	623	0	SER	Α	83	52.958	46.920	10.566	1.00 40.82	0
ATOM	624	CB	SER	Α	83	53.816	48.590	12.549	1.00 40.01	С
ATOM	625	OG	SER	Α	83	55.077	48.281	11.989	1.00 42.73	0
ATOM	626	N	GLN	Α	84	52.034	45.385	11.934	1.00 42.84	N
ATOM	627	CA	GLN	Α	84	51.552	44.502	10.879	1.00 43.52	C
ATOM	628	С	GLN		84	50.500	43.599	11.524	1.00 44.66	C
ATOM	629	0	GLN		84	50.323	43.632	12.742	1.00 44.23	0
ATOM	630	CB	GLN		84	52.699	43.665	10.310	1.00 43.55	С
ATOM	631	CG	GLN		84	53.361	42.741	11.318	1.00 43.62	С
ATOM	632	CD	GLN		84	54.467	41.917	10.694	1.00 45.55	C
			GLN		84	54.266	41.275		1.00 46.16	0
ATOM	633					55.646	41.926	11.319	1.00 44.86	N
ATOM	634		GLN SER		84 85	49.807	42.798	10.720	1.00 46.26	Ń
ATOM	635	N CA			85	48.774	41.912	11.249	1.00 47.95	Ĉ. C
ATOM	636		SER			49.364	40.964	12.283	1.00 47.55	C
ATOM	637	C	SER		85			12.239	1.00 48.83	0
ATOM	638	0	SER		85	50.554	40.648	10.128	1.00 47.83	C
ATOM	639	CB	SER		85	48.135	41.087		1.00 47.83	0
ATOM	640	OG	SER		85	48.937	39.965	9.804	1.00 48.77	
ATOM	641	N	ILE		86	48.520	40.517	13.209		N
ATOM	642	CA	ILE		-86		39.593	14.256	1.00 50.14	C
ATOM	643	C	ILE		86	49.416	38.281	13.636	1.00 51.13	C
MOTA	644	0	ILE		86	50.425	37.715	14.059	1.00 50.51	0
ATOM	645	CB	ILE		86	47.764	39.305	15.222	1.00 49.46	C
ATOM	646	CG1			86	47.346	40.605	15.919	1.00 49.50	C
MOTA	647		ILE		86	48.162	38.236	16.227	1.00 48.57	C
MOTA	648		ILE		86	46.160	40.463	16.864	1.00 49.15	C
ATOM	649	N	GLU		87	48.689	37.811	12.626	1.00 52.14	N
ATOM	650	CA	GLU		87	49.028	36.573	11.930	1.00 53.33	C
MOTA	651	C	GLU		87	50.377	36.714	11.227	1.00 52.06	C
MOTA	652	0	GLU	Α	87	51.197	35.795	11.228	1.00 51.76	0
MOTA	653	CB	GLU	Α	87	47.956	36.237	10.881	1.00 55.49	C
MOTA	654	CG	GLU	А	87	46.545	35.978	11.430	1.00 59.83	С
MOTA	655	CD	GLU	A	87	45.948	37.179	12.164	1.00 62.66	С
MOTA	656	OE1	GLU	А	87	45.934	38.298	11.594	1.00 63.16	0
ATOM	657	OE2	GLU	Α	87	45.484	36.998	13.314	1.00 64.49	0
ATOM	658	N	SER	Α	88	50.594	37.876	10.623	1.00 51.42	N
MOTA	659	CA	SER	Α	88	51.828	38.149	9.895	1.00 51.37	C
ATOM	660	C	SER	Α	88	53.048	38.223	10.818	1.00 49.76	C
MOTA	661	0	SER	A	88	54.098	37.651	10.522	1.00 48.93	0
ATOM	662.	CB	SER	Α	88	51,683	39.459	9.116	1.00 52.05	C
ATOM	663	OG	SER	Α	88	52.784	39.661	8.253	1.00 54.78	0
MOTA	664	N	GLN	Α	89	52.909	38.927	11.935	1.00 48.17	N
ATOM	665	CA	GLN	Α	89	54.010	39.051	1,2.878	1.00 47.23	C
ATOM	666	C	GLN	A	89	54.338	37.692	13.493	1.00 47.15	C
ATOM	667	0	GLN	A	89	55.507	37.333	13.636	1.00 47.13	0
MOTA	668	CB	GLN	A	89	53.663	40.060	13.980	1.00 45.26	C
ATOM	669	CG	GLN	A	89	54.718	40.149	15.081	1.00 43.42	С
ATOM	670	CD	GLN	A	89	54.405	41.207	16.127	1.00 42.17	C
MOTA	671	OE1	GLN	A	89	53.243	41.438	16.470	1.00 40.51	. 0
ATOM	672		GLN		89	55.447	41.840	16.658	1.00 40.16	N
ATOM	673	N	ALA		90	53.305	36.934	13.848	1.00 47.23	N
ATOM	674	CA	ALA		90	53.498	35.616	14.445	1.00 47.19	C
ATOM	675	С	ALA		90	54.224	34.678	13.486	1.00 47.12	C
ATOM	676	0	ALA		90	55.065	33.881	13.903	1.00 48.12	0
ATOM	677	СВ	ALA		90	52.154	35.022	14.848	1.00 47.65	C
ATOM	678	N	ALA		91	53.909	34.774	12.199	1.00 46.68	N
ATOM	679	CA	ALA		91	54.560	33.924	11.211	1.00 47.00	С
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ATOM	680	C	ALA	A	91	56.064	34.212	11.175	1.00 4	7.22		C
ATOM	681	0	ALA	Α	91	56.877	33.291	11.081	1.00 4	7.71		0
MOTA	682	CB	ALA	A	91	53.940	34.142	9.828	1.00 4	5.18		C
ATOM	683	N	MET	A	92	56.439	35.486	11.249	1.00 4	7.06		N
MOTA	684	CA	MET	A	92	57.856	35.840	11.237	1.00 4			C
MOTA	685	C	MET		92	58.568	35.257	12.451	1.00 4			C
ATOM	686	0	MET		92	59.684	34.753	12.340	1.00 4			0
ATOM	687	СВ	MET		92	58.041	37.357	11.222	1.00 4		•	C
ATOM	688	CG	MET		92	57.871	37.987	9.863	1.00 4			C
ATOM	689	SD	MET		92	58.254	39.733	9.915	1.00 4			s
ATOM	690	CE	MET		92	56.986	40.381	8.852		6.35		C
ATOM	691	N	VAL		93	57.925	35.333	13.611	1.00 4			N
ATOM	692	CA .	VAL		93	58.511	34.796	14.829	1.00 4			
ATOM	693	CA	VAL		93							C
ATOM	694	0	VAL			58.675	33.290	14.682	1.00 4			C
					93	59.715	32.733	15.037	1.00 4			0
ATOM	695	CB	VAL		93	57.624	35.090	16.057	1.00 4			C
ATOM	696		VAL		93	58.080	34.254	17.251	1.00 43			C
ATOM	697		VAL		93	57.692	36.568	16.394	1.00 4			C
MOTA	698	N	HIS		94	57.642	32.637	14.153	1.00 4			N
MOTA	699	CA	HIS		94	57.668	31.189	13.955	1.00 4	9.55		С
ATOM	700	C	HIS	Α	94	58.818	30.791	13.035	1.00 48	8.88		С
MOTA	701 ·	0	HIS	А	94	59.572	29.862	13.330	1.00 4	9.22		0
MOTA	702	CB	HIS	Α	94	56.344	30.703	13.349	1.00 5	1.41		С
MOTA	703	CG	HIS	Α	94	56.256	29.213	13.221	1.00.5	3.19		С
MOTA	704	ND1	HIS	Α	94	55.924	28.394	14.278	1.00 5	3.72		N
MOTA	705	CD2	HIS	Α	94	56.520	28.391	12.176	1.00 5	4.01		С
ATOM	706		HIS		94	55.989	27.131	13.893	1.00 5			C
ATOM	707		HIS		94	56.351	27.102	12.622	1.00 5			N
ATOM	708	N	ALA		95	58.952	31.502	11.921	1.00 48			N
ATOM	709	CA	ALA		95	60.006	31.219	10.956	1.00 4			C
ATOM	710	C	ALA		95	61.405	31.321	11.567	1.00 4			C
ATOM	711	0	ALA		95	62.294	30.538	11.233	1.00 4			0
ATOM	712	CB	ALA		95	59.887	32.162	9.770	1.00 4			C
ATOM	713	N	VAL		96	61.604	32.162	12.458	1.00 4			
		CA	VAL									N
ATOM	714				96	62.906	32.463	13.087	1.00 4			C
ATOM	715	C	VAL		96	63.165	31.344	14.086	1.00 48			C
ATOM .	716	0	VAL		96	64.276	30.815	14.164	1.00 4			0
ATOM	717	CB	VAL		96	63.003	33.826	13.815	1.00 4	•		C
ATOM	718		VAL		96	64.336	33.945	14.537	1.00 4			C
MOTA	719		VAL		96	62.856	34.952	12.813	1.00 4			С
ATOM	720	N	LYS		97	62.133	30.979	14.840	1.00 48			N
MOTA	721	CA	LYS		97	62.252	29.924	15.837	1.00 5			С
MOTA	722	С	LYS		97	62.459	28.546	15.209	1.00 5	2.32		C
ATOM	723	0	LYS		97	63.068	27,.670	15.823	1.00 5			0
ATOM	724	CB	LYS		97	61.010	29.899	16.742	1.00 49	9.44		С
ATOM	725	CG	LYS	·A	97	60.791	31.169	17.564	1.00 4	7.42		С
ATOM	726	CD	LYS	Α	97	61.988	31.489	18.467	1.00 4	5.88		С
ATOM	727	CE	LYS	Α	97	62.191	30.440	19.557	1.00 44	1.36		C
ATOM	728	NZ	LYS	Α	97	63.433	30.692	20.354	1.00 42	2.11		N
ATOM	729	N	ASN		98	61.962	28.354	13.991	100 54			N
ATOM	730	CA	ASN		98	62.108	27.066	13.315	1.00 58			С
ATOM	731	С	ASN		98	63.004	27.120	12.085	1.00 59			C
ATOM	732	0	ASN		98	62.799	26.361	11.138	1.00 60			o
ATOM	733	CB	ASN		98	60.738	26.515	12.899	1.00 58			C
	734	CG	ASN		98	59.882	26.119	14.082	1.00 6			C
ATOM	735		ASN		98	59.420	26.970	14.845	1.00 6			0
ATOM	736		ASN		98	59.668	24.816	14.248	1.00 62			И
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ATOM	737	N	PHE .	А	99	64.000	27.999	12.092	1.00	61.00		N
MOTA	738		PHE		99	64.889	28.117	10.942	1.00	62.73		С
ATOM	739	C	PHE		99	65.827	26.926	10.774	1.00	64.62		C
ATOM	740	0	PHE		99	66.150	26.544	9.650	1.00	64.73		0
ATOM	741	CB	PHE		99	65.719	29.398	11.028	1.00	61.76		C
ATOM	742	CG	PHE		99	66.492	29.703	9.772	1.00	61.06		С
ATOM	743		PHE		99	65.827	29.971	8.579		60.96		С
ATOM	744		PHE		99	67.881	29.727	9.780	1.00	60.81		C
ATOM	745		PHE		99	66.537	30.258	7.412		60.52		C
ATOM	746		PHE		99	68.599	30.012	8,620		60.86		C
ATOM	747	CZ	PHE		99	67.924	30.279	7.434		60.69		C
	748	N	LYS			66.267	26.340	11.883		67.08	•	N
ATOM ATOM	749	CA	LYS			67.178	25.199	11.820		70.33	•	C
	750	C	LYS			66.462	23.871	11.582		72.95		С
ATOM	751	0	LYS			66.988	22.809	11.914		72.97		0
ATOM	752	CB	LYS			68.006	25.108	13.104		69.54	•	С
ATOM	753	CG	LYS			68.932	26.288	13.333		68.73		С
ATOM		CD	LYS			69.765	26.088	14.586		68.36		C ·
ATOM	754	CE	LYS			70.750	27.227	14.791		67.27		С
MOTA	755 756	NZ	LYS			71.581	27.006	16.000		66.23		N
ATOM	756	N N	ALA			65.269	23.937	10.999		76.17		N
ATOM	7.57	CA	ALA			64.486	22.739	10.717		79.28		C
MOTA	758		ALA			64.671	22.262	9.275		81.72		C
ATOM	759	C	ALA			65.159	21.154	9.043		81.99		0
ATOM	760	O	ALA			63.139	23.002	10.996		79.19		C
ATOM	761	CB	GLY			64.280	23.092	8.310		84.33		N
ATOM	762	N				64.420	22.707	6.915		87.56		C
ATOM	763	CA	GLY			63.773	23.645	5.910		89.81		Ċ
ATOM	764	C	GLY			62.728	24.243	6.179		90.05		Ō
ATOM	765	0	GLY			64.402	23.760	4.741		91.88		N
ATOM	766	N	PHE			63.930	24.618	3.653		93.97		C
ATOM	767	CA	PHE			62.785	23.976	2.864		95.19		C
ATOM	768	C	PHE			61.854	24.661	2.427		95.10		o
ATOM	769	0	PHE			65.107	24.933	2.714		94.40		C
ATOM	770	CB	PHE			64.716	25.637	1.439		95.36		C
ATOM	771	CG	PHE			64.030	24.961	0.430		95.96		C
ATOM	772		PHE			65.052	26.973	1.238		95.68		C
ATOM	773		PHE			63.682	25.603	-0.758		96.63		C
ATOM	774		PHE			64.710	27.627	0.054		96.41		C
MOTA	775	CEZ			103	64.024	26.940	-0.947		96.90		C
MOTA	776		"VAL			62.867	22.660	2.685		96.51		N
ATOM	777				104	61.864	21.904	1.941		97.40		C
ATOM	778	CA C			104	60.668	21.484	2.796		98.06		С
ATOM	779				104	60.475	21.986	3.905		98.29		0
ATOM	780 701	O CB			104	62.494	20.639	1.318		97.53		C
ATOM	781		VAL			63.604	21.035	0.358		97.83		C
MOTA	782		VAL			63.043	19.733	2.415		97.17		С
MOTA	783	N CG2			105	59.869	20.562	2.265		98.68		N
ATOM	784				105	58.690	20.055	2.960		99.19		C
ATOM	785	·CA			105	58.840	18.556	3.223		99.69		Ċ
ATOM	786	C			105	59.955	18.034	3.251		99.86		Ō
MOTA	787	O				, 57.408	20.294	2.130		99.21		Ċ
ATOM	788	CB			105	57.207	21.786	1.904		98.66		Ċ
ATOM	789		VAL			57.505	19.562	0.798		99.13		Ċ
ATOM	790		VAL			57.720	17.864	3.411		100.19		N
ATOM	791	N			106	57.748	16.427	3.674		100.80		C
ATOM	792	CA			106		15.604	2.401		0101.31		Ċ
MOTA	793	C	SER	A	106	57.538	15.004	2.401	1.00	,		_

ATOM	794	0	SER	Α	106	56.616	14.788	2.323	1.00101.42		0
ATOM	795	CB	SER .	Α	106	56.678	16.063	4.707	1.00100.69		C
ATOM	796	OG	SER	Α	106	55.384	16.412	4.245	1.00100.34		0
ATOM	797	N	ASP	Α	107	58.402	15.816	1.412	1.00101.66		N
ATOM	798	CA	ASP	A	107	58.312	15.101	0.142	1.00101.66		C
MOTA	799	C	ASP	A	107	59.084	13.785	0.184	1.00101.55		С
MOTA	800	0	ASP	Α	107	59.050	13.003	-0.767	1.00101.37		0
MOTA	801	CB	ASP	Α	107	58.848	15.976	-0.997	1.00101.95		С
MOTA	802	CG	ASP	Α	107	60.326	16.302	-0.843	1.00102.22		C
ATOM	803	OD1	ASP	Α	107	60.742	16.916	0.140	1.00102.16		0
ATOM	804	OD2	ASP	Α	107	61.126	15.891	-1.821	1.00102.12		0
MOTA	805	N	VAL	A	220	77.129	27.310	12.363	1.00 82.99		N
ATOM	806	CA	VAL	A	220	78.036	26.953	13.450	1.00 82.93		С
ATOM	807	C	VAL	Α	220	78.735	28.199	13.998	1.00 82.11		C
ATOM	808	0	VAL	Α	220	79.965	28.283	14.018	1.00 82.35		0
MOTA	809	CB	VAL	A	220	79.103	25.942	12.967	1.00 83.59		С
ATOM	810	CG1	VAL	Α	220	79.931	25.443	14.152	1.00 83.61		C
ATOM	811	CG2	VAL	Α	220	78.424	24.777	12.252	1.00 84.13		C
ATOM	812	N	CYS	A	221	77.936	29.165	14.439	1.00 80.94	Ý.,.	N
ATOM	813	CA	CYS	Α	221	78.454	30.414	14.989	1.00 79.61		С
ATOM	814	С	CYS	Α	221	78.548	30.290	16.509	1.00 78.38		C
ATOM	815	0	CYS	Α	221	77.557	29.996	17.176	1.00 78.27		0
ATOM	816	CB	CYS	Α	221	77.526	31.568	14.602	1.00 80.09		С
ATOM	817	SG	CYS	Α	221	77.159	31.648	12.823	1.00 80.23		S
MOTA	818	N	HIS	A	222	79.739	30.518	17.054	1.00 76.79		N
ATOM	819	CA	HIS	Α	222	79.949	30.395	18.493	1.00 74.99		C
MOTA	820	С	HIS	Α	222	79.364	31.496	19.366	1.00 72.24		С
ATOM	821	0	HIS	Α	222	79.359	31.376	20.592	1.00 72.13		0
MOTA	822	CB	HIS	Α	222	81.442	30.238	18.799	1.00 77.56		C
MOTA	823	CG	HIS	Α	222	81.952	28.846	18.586	1.00 80.75		С
MOTA	824	ND1	HIS			81.352	27.741	19.155	1.00 81.58		N
MOTA	825	CD2	HIS	Α	222	83.003.	28.377	17.872	1.00 81.49		С
ATOM	826	CE1	HIS	Α	222	82.011	26.653	18.799	1.00 82.43		С
ATOM	827	NE2	HIS	Α	222	83.017	27.011	18.021	1.00 82.72		N
ATOM	828	N	ASN	Α	223	78.875	32.565	18.751	1.00 68.37		N
MOTA	829	CA	ASN	А	223	78.282	33.643	19.526	1.00 64.96		C
ATOM	830	C	ASN	Α	223	76.793	33.775	19.261	1.00 61.91		С
ATOM	831	0	ASN	Α	223	76.185	34.788	19.599	1.00 60.48		0
MOTA	832	CB	ASN	Α	223	78.984	34.968	19.237	1.00 65.81		C
MOTA	833	CG	ASN	A	223	80.285	35.107	19.998	1.00 66.63		C
MOTA	834	OD1	ASN	A	223	80.302	35.069	21.229	1.00 65.69		0
MOTA	835	ND2	ASN	A	223	81.385	35.266	19.270	1.00 67.36		N
MOTA	836	N	GLU	A	224	76.206	32.746	18.660	1.00 58.19		N
MOTA	837	CA	GLU	Α	224	74.780	32.774	18.371	1.00 55.64		C
ATOM	838	C	GLU	Α	224	73.972	32.796	19.657	1.00 51.83		C
MOTA	839	0	GLU	Α	224	74.341	32.166	20.646	1.00 50.93	•	0
MOTA	840	CB	GLU	Α	224	74.36 <b>7</b>	31.560	17.534	1.00 56.74		C
MOTA	841	CG	GLU	Α	224	74.747	30.220	18.136	1.00 59.42		C
MOTA	842	CD	GLU	Α	224	74.114	29.053	17.398	1.00 60.69		C
MOTA	843		GLU			74.019	29.115	16.149	1.00 61.36	•	0
MOTA	844	OE2	GLU	A	224	73.722	28.073	18.069	1.00 60.59		0
MOTA	845	N	LEU	Α	225	72.871	33.536	19.634	1.00 48.65		N
MOTA	846	CA			225	71.991	33.641	20.785	1.00 46.12		C
MOTA	847	C	LEU	Α	225	70.843	32.660	20.571	1.00 44.98		C
MOTA	848	0	LEU	Α	225	70.031	32.832	19.660	1.00 42.50		0
MOTA	849	CB	LEU	A	225	71.456	35.071	20.904	1.00 45.35		C
ATOM	850	CG	LEU	A	225	70.635	35.402	22.151	1.00 46.02		С

ATOM	851	CD1	LEU	Α	225	71.483	35.146	23.389	1.00 46.56	С
MOTA	852	CD2	LEU	Α	225	70.174	36.851	22.107	1.00 45.65	C
ATOM	853	N	VAL	Α	226	70.778	31.634	21.415	1.00 45.11	N
ATOM	854	CA	VAL			69.740	30.612	21.293	1.00 45.18	C
ATOM	855	C	VAL			69.138	30.162	22.623	1.00 46.10	. С
ATOM	856	0	VAL			69.664	30.461	23.698	1.00 46.22	0
ATOM	857	CB.	VAL			70.294	29.355	20.598	1.00 44.37	С
ATOM	858		VAL			70.698	29.674	19.170	1.00 42.78	С
ATOM	859		VAL			71.478	28.826	21.383	1.00 43.24	С
			ASP			68.026	29.435	22.535	1.00 46.56	N
ATOM	860	N CA	ASP			67.366	28.912	23.721	1.00 47.21	C
ATOM	861					67.910	27.516	24.017	1.00 48.24	C
ATOM	862	C	ASP ASP			68.808	27.034	23.325	1.00 47.45	Ō
ATOM	863	O					28.854	23.523	1.00 46.83	C
ATOM	864	CB	ASP			65.848		22.264	1.00 46.84	C
MOTA	865	CG	ASP			65.445	28.110	21.924	1.00 47.01	0
ATOM	866		ASP			66.094	27.099		1.00 47.01	o
MOTA	867		ASP			64.460	28.529	21.620		N
MOTA	868	N	SER			67.357	26.875	25.043	1.00 50.32	. C
MOTA	869	CA	SER			67.782	25.541	25.456	1.00 52.29	
ATOM	870	C	SER			67.580		24.366	1.00 53.54	. C
MOTA	871	0	SER			68.129	23.386	24.448	1.00 54.15	0
MOTA	872	CB	SER			67.031	25.127	26.723	1.00 51.85	C
MOTA	873	OG			228	65.636	25.099	26.492	1.00 52.33	0
ATOM	874	N			229	66.793	24.832	23.352	1.00 54.18	N
ATOM	875	CA	GLN	Α	229	66.526	23.934	22.237	1.00 54.92	C
ATOM	876	С	GLN	Α	229	67.418	24.282	21.049	1.00 55.01	C
ATOM	877	0	GLN	Α	229	67.224	23.772	19.942	1.00 55.05	0
ATOM	878	CB	GLN	Α	229	65.058	24.038	21.818	1.00 56.21	C
ATOM	879	CG	GLN	Α	229	64.088	23.265	22.691	1.00 58.02	C
MOTA	880	CD	GLN	Α	229	62.641	23.613	22.386	1.00 60.19	C
ATOM	881	OE1	GLN	Α	229	62.130	24.637	22.845	1.00 60.85	0
ATOM	882	NE2	GLN	Α	229	61.976	22.770	21.597	1.00 61.03	N
ATOM	883	N	LYS	A	230	68.392	25.157	21.287	1.00 54.58	N
ATOM	884	CA			230	69.328	25.596	20.255	1.00 53.47	C
ATOM	885	C			230	68.684	26.418	19.137	1.00 51.87	C
ATOM	886	0			230	69.257	26.554	18.055	1.00 51.62	0
ATOM	887	CB			230	70.057	24.390	19.652	1.00 55.91	C
ATOM	888	CG			230	70.846	23.572	20.669	1.00 58.78	C
	889	CD			230	71.977	24.381	21.305	1.00 61.46	C
ATOM	890				230	73.062	24.738		1.00 62.75	C
ATOM	891	NZ			230	74.211	25.454	20.926	1.00 63.92	N
MOTA	892	N			231	67.501	26.970	19.395	1.00 50.44	N
MOTA	893	CA			231	66.816	27.796	18.400	1.00 48.86	С
ATOM	894	C			231	67.179	29.261	18.644	1.00 47.36	. С
MOTA	895	0			231	67.351	29.679	19.789	1.00 45.45	0
		СВ			231	65.296	27.637	18.512	1.00 50.40	C
MOTA	896				231	64.794	26.199	18.451	1.00 51.58	C
ATOM	897	CG			231	63.779	25.952	19.553	1.00 53.03	C
MOTA	898	CD					26.504	19.257	1.00 55.50	N
ATOM	899	NE			231	62.461			1.00 56.77	C
ATOM	900	CZ			231	61.573	26.852	20.186 21.471	1.00 57.45	N
MOTA	901				231	61.869	26.716			N
MOTA	902				231	60.379	27.317	19.833	1.00 57.86	N
MOTA	903	N			232	67.294	30.034	17.567	1.00 45.64	C
ATOM	904	CA			232	67.623	31.450	17.671	1.00 43.85	
MOTA	905	C			232	66.581	32.200	18.497	1.00 42.80	C
ATOM	906	0			. 232	65.376	31.965	18.361	1.00 41.87	0
MOTA	907	CB	TYR	A	232	67.692	32.093	16.286	1.00 43.80	C

ATOM	908	CG	TYR .	A	232	68.821	31.603	15.423	1.00 44.82	C
ATOM	909	CD1	TYR .	A	232	70.142	31.650	15.871	1.00 45.02	C
MOTA	910	CD2	TYR .	Α	232	68.573	31.094	14.151	1.00 45.58	C
ATOM	911 .	CE1	TYR .	Α	232	71.193	31.197	15.066	1.00 46.46	C
ATOM	912	CE2	TYR	Α	232	69.610	30.642	13.341	1.00 46.70	C
ATOM	913	CZ	TYR	Α	232	70.915	30.694	13.803	1.00 46.56	C
MOTA	914	OH	TYR	Α	232	71.932	30.237	12.998	1.00 47.52	0
ATOM	915	N	LEU	Α	233	67.044	33.097	19.358	1.00 41.20	N
MOTA	916	CA	LEU	Α	233	66.119	33.882	20.160	1.00 40.26	C
ATOM	917	Ċ	LEU	Α	233	65.573	34.990	19.275	1.00 39.17	C
ATOM	918	0	LEU	Α	233	66.231	35.428	18.328	1.00 39.41	0
ATOM	919	CB	LEU	Α	233	66.816	34.493	21.380	1.00 39.71	C
ATOM	920	CG	LEU	Α	233	67.335	33.532	22.453	1.00 40.47	С
ATOM	921	CD1	LEU	A	233	67.794	34.339	23.661	1.00 40.88	C
ATOM	922	CD2	LEU	Α	233	66.243	32.562	22.870	1.00 39.44	С
ATOM	923	N	VAL			64.360	35.432	19.572	1.00 37.75	N
ATOM	924	CA	VAL	A	234	63.756	36.498	18.799	1.00 37.14	C
ATOM	925	С	VAL	Α	234	62.766	37.241	19.681	1.00 37.43	С
ATOM	926	0	VAL	А	234	62.157	36.653	20.575	1.00 37.88	0
ATOM	927	CB	VAL	А	234	63.032	35.946	17.544	1.00 36.92	C
MOTA	928	CG1	VAL	Α	234	61.826	35.102	17.954	1.00 34.91	C
ATOM	929	CG2	VAL	Α	234	62.619	37.096	16.638	1.00 35.20	C
ATOM	930	N	GLY	Α	235	62.631	38.540	19.444	1.00 36.87	N
MOTA	931	CA	GLY	A	235	61.703	39.335	20.223	1.00 36.91	С
MOTA	932	С	GLY	Α	235	60.596	39.828	19.318	1.00 36.80	. C
ATOM	933	0	GLY	Α	235	60.670	39.654	18.098	1.00 37.13	0
ATOM	934	N	ALA	Α	236	59.572	40.440	19.903	1.00 35.88	N
MOTA	935	CA	ALA	A	236	58.465	40.958	19.116	1.00 35.95	C
MOTA	936	С	ALA	A	236	57.824	42.165	19.791	1.00 35.70	C
MOTA	937	0	ALA	Α	236	57.559	42.153	20.995	1.00 37.71	0
ATOM	938	CB	ALA	Α	236	57.423	39.860	18.893	1.00 36.04	C
ATOM	939	N	GLY	A	237	57.578	43.212	19.012	1.00 35.37	N
MOTA	940	CA	$\operatorname{GLY}$	A	237	56.961	44.401	19.564	1.00 36.75	C
MOTA	941	C	GLY	Α	237	55.459	44.243	19.696	1.00 38.21	C
MOTA	942	0	GLY	А	237	54.837	43.542	18.895	1.00 39.76	0
MOTA	943	N	ILE	Α	238	54.876	44.870	20.715	1.00 36.81	. N
MOTA	944	CA	ILE	Α	238	53.437	44.818	20.926	1.00 37.17	C
MOTA	945	C	ILE	A	238	52.933	46.227	21.232	1.00 37.51	C
MOTA	946	0	ILE	Α	238	53.713	47.111	21.591	1.00 36.78	0
MOTA	947	CB			238	53.043	43.883	22.107	1.00 38.27	C
MOTA	948		ILE			53.568	44.449	23.432	1.00 38.61	C
ATOM	949		ILE			53.588		21.872	1.00 36.69	C
MOTA	950	CD1	ILE			53.046	43.710	24.665	1.00 38.14	C
MOTA	951	N			239	51.631		21.074	1.00 37.56	N
MOTA	952	CA			239	51.048		21.351	1.00 37.15	C C
MOTA	953	C			239	50.037		22.484	1.00 38.42	
MOTA	954	0			239	49.644		22.873	1.00 37.39	0
MOTA	955	CB			239	50.388		20.090	1.00 37.73	C
MOTA	956	CG			239	49.255		19.575	1.00 38.01	
MOTA	957		ASN			48.224		20.228	1.00 37.30	N C
MOTA	958		ASN			49.446		18.402	1.00 37.32	N
MOTA	959	N			240	49.629		23.018	1.00 39.33	C
MOTA	960	CA			240	48.678		24.121	1.00 40.33	C
ATOM	961	C			240	47.219		23.672	1.00 42.53	C
MOTA	962	0			240	46.299		24.468	1.00 41.92	
ATOM	963	CB			240	48.812		24.870	1.00 39.24	
MOTA	964	OG1	THR	A	240	48.634	51.242	23.940	1.00 39.26	

ATOM	965	CG2	THR	A	240 -	50.192	50.293	25.514	1.00 37.80		C
ATOM	966	N	ARG	A	241	47.010	48.319	22.409	1.00 44.79		N
MOTA	967		ARG			45.659	48.177	21.876	1.00 48.48		C
MOTA	968	C	ARG			45.165	46.738	21.739	1.00 48.69		C
ATOM	969	Ō	ARG			44.291	46.305	22.487	1.00 48.51	•	0
ATOM	970	СВ	ARG			45.565	48.862	20.509	1.00 51.38		C
	971	CG	ARG			45.987	50.327	20.508	1.00 56.77		С
MOTA	972	CD	ARG			44.854	51.258	20.917	1.00 60.32		С
MOTA		NE	ARG			43.743	51.209	19.965	1.00 63.77		N
ATOM	973					42.827	52.166	19.829	1.00 65.29		C
ATOM	974	CZ	ARG			42.885	53.260	20.583	1.00 65.45		N
MOTA	975		ARG					18.939	1.00 65.16		N
MOTA	976	NH2	ARG			41.850	52.030	20.781	1.00 48.65		N
MOTA	977	N	ASP			45.724	46.006		1.00 48.03		C
MOTA	978	CA	ASP			45.304	44.632	20.523			C
MOTA	979	С	ASP			46.142	43.558	21.206	1.00 50.06		0
MOTA	980	0	ASP			46.237	42.442	20.702	1.00 51.04		
MOTA	981	CB	ASP			45.306	44.362	19.013	1.00 49.94		C
MOTA	982	CG	ASP	A	242	46.696	44.458	18.404	1.00 51.08		C
MOTA	983	OD1	ASP	А	242	47.683	44.268	19.146	1.00 50.09		0
MOTA	984	OD2	ASP	А	242	46.804	44.708	17.181	1.00 51.20		0
MOTA	985	N	PHE	Α	243	46.732	43.879	22.353	1.00 49.77		N
MOTA	986	CA	PHE	Α	243	47.579	42.924	23.065	1.00 49.06		C
ATOM	987	С	PHE	A	243	46.889	41.647	23.549	1.00 49.87		С
ATOM	988	0	PHE	Α	243	47.539	40.609	23.694	1.00 49.78		0
MOTA	989	CB	PHE	А	243	48.274	43.617	24.242	1.00 45.99	-	C
ATOM	990	CG	PHE	Α	243	47.334	44.151	25.279	1.00 44.15	•	C
ATOM	991	CD1	PHE			46.841	43.323	26.283	1.00 43.69		C
ATOM	992		PHE			46.956	45.490	25.268	1.00 43.83		C
ATOM	993		PHE			45.989	43.821	27.266	1.00 42.27		C
MOTA	994		PHE			46.103	46.001	26.247	1.00 43.52		C
ATOM	995	CZ	PHE			45.619	45.163	27.249	1.00 43.49		С
ATOM	996	N	ARG			45.583	41.714	23.796	1.00 50.68		N
	997	CA			244	44.852	40.537	24.260	1.00 51.51		С
MOTA			ARG			44.820	39.453	23.187	1.00 51.28		C
ATOM	998	C				44.620	38.268	23.494	1.00 51.51		0
ATOM	999	0	ARG			43.423		24.682	1.00 52.01		C
ATOM	1000	CB			244		40.915		1.00 52.37		C
MOTA	1001	CG			244	43.368	41.841	25.899	1.00 52.37		C
MOTA	1002	CD			244	41.939	42.089	26.374	1.00 53.17		N
MOTA	1003	NE			244	41.895	43.054	27.473			C
MOTA	1004		ARG		and the second second		44.359	27.337	1.00 55.49		-
MOTA	1005		ARG			42.408	44.870	26.144	1.00 54.46		N
MOTA	1006	NH2	ARG			42.089	45.154	28.399	1.00 55.06		N
MOTA	1007	N	GLU	Α	245	44.935	39.859	21.928	1.00 50.95		N
MOTA	1008	CA	GLU	Α	245	44.940	38.906	20.826	1.00 51.31		C
MOTA	1009	С	GLU	Α	245	46.362	38.666	20.335	1.00 50.29		C
MOTA	1010	0	GLU	Α	245	46.770	37.526	20.107	1.00 50.46		0
MOTA	1011	CB	GLU	A	245	44.095	39.415	19.653	1.00 53.93		С
ATOM	1012	CG	GLU	Α	245	42.588	39.248	19.813	1.00 58.44		. C
MOTA	1013	CD	GLU	Α	245	42.012	40.073	20.950	1.00 61.81		С
MOTA	1014		GLU			42.234	41.309	20.972	1.00 63.52		0
MOTA	1015		GLU			41.329	39.484	21.818	1.00 63.32		0
MOTA	1016	N			246	47.117	39.749	20.181	1.00 48.30		N
ATOM	1017	CA			246	48.489	39.671	19.689	1.00 46.47		C
ATOM	1018	C			246	49.447	38.897	20.599	1.00 45.04		С
MOTA	1019	0			246		38.036	20.132	1.00 44.61		0
ATOM	1019	СВ			246	49.029	41.085	19.442	1.00 45.89		C
		CG			246	50.345	41.127	18.681	1.00 45.20		C
ATOM	1021	CG	ARG	А	440	50.345	T1.14/	10.001	1.00 40.20		~

MOTA	1022	CD	ARG	А	246	50.833	42.556	18.513	1.00	44.73		С
MOTA	1023	NE	ARG	Α	246	49.950	43.359	17.671	1.00	43.18		N
MOTA	1024	CZ	ARG	Α	246	49.880	43.265	16.347	1.00	42.54		С
MOTA	1025	NH1	ARG	Α	246	50.644	42.402	15.694	1.00	41.20		N
MOTA	1026		ARG			49.042	44.040	15.673	1.00	44.27		N
ATOM	1027	N	VAL			49.435	39.193	21.894	1.00	44.31		N
MOTA	1028	CA	VAL			50.335	38.509	22.819	1.00	44.71		С
ATOM	1029	C	VAL			50.238	36.976	22.757		45.57		С
ATOM	1030	0	VAL			51.245	36.296	22.530		45.24		0
	1030	CB	VAL			50.101	38.984	24.274		43.46		C
MOTA							38.123	25.244		43.08		C
ATOM	1032					50.894		24.410		43.85		C
ATOM	1033		VAL			50.512	40.444					N
MOTA	1034	N			248	49.027	36.411	22.959		45.51		C
MOTA	1035	CA			248	48.879	34.952	22.912`		44.41		
ATOM	1036	C			248	49.439	34.367	21.624		44.05		C
MOTA	1037	0			248	50.118	33.348	21.641		44.00		0
ATOM	1038	CB			248	47.369	34.755	23.030		45.34		C
MOTA	1039	CG			248	46.956	35.899	23.898		45.42		C
MOTA	1040	CD			248	47.741	37.052	23.297		44.89		С
MOTA	1041	N	ALA	Α	249	49.162	35.028	20.508	1.00	43.48		N
MOTA	1042	CA	ALA	Α	249	49.639	34.565	19.215	1.00	43.34		C
ATOM	1043	C	ALA	A	249	51.167	34.583	19.129	1.00	44.16		C
MOTA	1044	0	ALA	Α	249	51.774	33.705	18.504	1.00	43.00		0
MOTA	1045	CB	ALA	A	249	49.040	35.421	18.111	1.00	42.95		C
ATOM	1046	N	LEU	A	250	51.786	35.582	19.755	1.00	43.64		N
ATOM	1047	CA	LEU	Α	250	53.238	35.692	19.729	1.00	43.74		С
ATOM	1048	С	LEU	Α	250	53.862	34.647	20.643	1.00	43.57		С
ATOM	1049	0			250	54.897	34.069	20.322	1.00	41.77		0
ATOM	1050	CB			250	53.677	37.110	20.125	1.00	43.33		С
ATOM	1051	CG			250	53.303	38.171	19.078	1.00	43.68		С
ATOM	1052				250 ·	53.687	39.554	19.563	1.00	43.65		С
ATOM	1053		LEU			54.001	37.858	17.761	1.00	42.84		С
ATOM	1054	N			251	53.223	34.398	21.778	1.00	44.52		N
MOTA	1055	CA			251	53.721	33.398	22.708	1.00	47.01		C
ATOM	1056	С			251	53.668	32.020	22.049	1.00	48.22		С
ATOM	1057	0			251	54.659	31.289	22.047	1.00	48.12		0
ATOM	1058	CB			251	52.883	33.364	23.993	1.00	47.37		С
ATOM	1059	CG1			251	53.327	32.206	24.870		48.76		C
ATOM	1060		VAL			53.031	34.678	24.739	1.00	48.75		С
ATOM	1061	N			252	52.512	31.676	21.483		49.02		N
ATOM	1062	CA			252	52.341	30.383	20.821		50.45		С
ATOM	1063	C			252	53.372	30.211	19.712		48.80		С
ATOM	1064	0			252	53.859	29.109	19.476		48.65		0
ATOM	1065	СВ			252	50.945	30.253	20.195		53.26		C
ATOM	1066	CG			.252	49.795	30.809	21.010		58.83		C
ATOM	1067	CD			252	49.648	30.175	22.379		62.50		C
	1067		GLU			48.721	30.596	23.108		64.11		Ō
ATOM						50.444	29.267	22.727		64.32		Ō
ATOM	1069		GLU			53.688	31.303	19.022		47.24		N
ATOM	1070	N			253		31.303	17.933		45.47		C
ATOM	1071	CA			253	54.658						C.
ATOM	1072	C			253	56.075	31.044	18.457		44.43	•	
ATOM	1073	0			253	56.988	30.749	17.686		43.74		0
ATOM	1074	CB			253	54.591	32.563	17.131		45.15		C
ATOM	1075	N			254	56.253	31.184	19.769		43.76		N
ATOM	1076	CA			254	57.562	30.968	20.366		43.81		C
ATOM	1077	C			254	58.415	32.207	20.610		43.78		0
MOTA	1078	0	لايلنى	A	254	59.635	32.103	20.751	1.00	43.49		U

MOTA	1079	N	ALA	A	255	57.793	33.381	20.658	1.00 4	2.53		N
ATOM	1080	CA	ALA	Α	255	58.540	34.611	20.902	1.00 4	0.96		С
ATOM	1081	C	ALA	Α	255	59.227	34.506	22.263	1.00 3	9.56		С
MOTA	1082	0	ALA	Α	255	58.595	34.154	23.260	1.00 4	0.08		0
ATOM .	1083	CB	ALA	Α	255	57.603	35.805	20.871	1.00 4	0.32		С
ATOM	1084	N	ASP			60.520	34.812	22.307	1.00 3	8.45		N
ATOM	1085	CA	ASP			61.274	34.723	23.557	1.00 3	8.35		С
ATOM	1086	C	ASP			61.088	35.928	24.478	1.00 3			C
ATOM	1087	0	ASP			61.159	35.802	25.700	1.00 3	6.65		0
ATOM	1088	СВ	ASP			62.752	34.522	23.247	1.00 3			С
ATOM	1089	CG	ASP			63.007	33.235	22.497	1.00 4			С
ATOM	1090		ASP			62.884	32.161	23.123	1.00 4			0
ATOM	1091	OD2				63.313	33.292	21.286	1.00 3			0
ATOM	1092	N	VAL			60.847	37.093	23.890	1.00 3		•	N
ATOM	1093	CA	VAL			60.647	38.302	24.676	1.00 3			C
ATOM	1094	C	VAL			59.773	39.278	23.903	1.00 3			C
ATOM	1095	0	VAL			59.755	39.265	22.678	1.00 3			0
	1095	CB	VAL			61.999	38.979	25.019	1.00 3			C
MOTA	1096		VAL			62.725	39.352	23.746	1.00 3			C
MOTA			VAL				40.206	25.889	1.00 3			C
ATOM	1098					61.771		24.626	1.00 3			N
MOTA	1099	N			258	59.040	40.113					
ATOM	1100	CA	LEU			58.173	41.095	23.993	1.00 3			C
ATOM	1101	C	LEU			58.597	42.498	24.423	1.00 3			C
MOTA	1102	0	LEU			59.376	42.661	25.359	1.00 3			0
MOTA	1103	CB	LEU			56.713	40.857	24.402	1.00 3			C
ATOM	1104	CG			258	56.155		24.206	1.00 3			C
ATOM	1105		LEU			54.719	39.402	24.682	1.00 3			C
ATOM	1106	CD2	LEU			56.245	39.027	22.747	1.00 3			C
MOTA	1107	N			259	58.100	43.509	23.721	1.00 3			N
ATOM	1108	CA			259	58.403	44.886	24.080	1.00 3			C
ATOM	1109	С			259	57.318	45.825	23.576	1.00 3			C
MOTA	1110	0	CYS	Α	259	57.033	45.867	22.377	1.00 3			0
ATOM	1111	CB	CYS	Α	259	59.756	45.329	23.512	1.00 3	4.49		C
MOTA	1112	SG	CYS	Α	259	60.296	46.925	24.191	1.00 3	4.45		S
MOTA	1113	N	ILE	Α	260	56.712	46.568	24.496	1.00 3	4.72		N
MOTA	1114	CA	ILE	Α	260	55.682	47.526	24.126	1.00 3	6.19		С
MOTA	1115	С	ILE	Α	260	56.391	48.632	23.350	1.00 3	7.93		C
MOTA	1116	0	ILE	Α	260	57.355	49.223	23.829	1.00 3	7.54		0
ATOM	1117	CB	ILE	А	260	55.003	48.122	25.364	1.00 3			C
ATOM	1118	CG1	ILE	Α	260	54.471	46.988	26.247	1.00 3	4.45		C
ATOM	1119	CG2	ILE	Α	260	53.868	49.052	24.937	1.00 3	4.98		С
ATOM	1120	CD1	ILE	Α	260	53.866	47.456	27.556	1.00 3	2.91		С
ATOM	1121	N	ASP	Α	261	55.905	48.886	22.143	1.00 3	9.60	*	N
ATOM	1122	CA	ASP	Α	261	56.472	49.873	21.236	1.00 4	0.88		C
MOTA	1123	C	ASP	Α	261	55.700	51.197	21.318	1.00 4	1.39		C
MOTA	1124	0	ASP	Α	261	54.549	51.275	20.887	1.00 4	2.16		0
ATOM	1125	СВ	ASP	Α	261	56.422	49.266	19.826	1.00 4	2.12		С
ATOM	1126	CG			261	56.977	50.179	18.756	1.00 4			С
ATOM	1127		ASP			57.842	51.025	19.061	1.00 4			0
ATOM	1128		ASP			56.553	50.025	17.591	1.00 4			0
ATOM	1129	N			262	56.328	52.232	21.881	1.00 4			N
ATOM	1130	CA			262	55.673	53.535	22.030	1.00 3			C
ATOM	1131	C			262	56.679	54.678	22.197	1.00 3			C
ATOM	1132	0			2,62	57.777	54.464	22.711	1.00 4			0
ATOM	1133	CB			262	54.733	53.492	23.242	1.00 4			C
ATOM	1134	OG			262	54.167	54.761	23.518	1.00 4			0
ATOM	1135	N			263	56.305	55.888	21.778	1.00 3			N
111011	1100	.,	אנייי	_	203	20.505	23.000		2.50 5	3.30		

ATOM	1136	CA	SER	Α	263	57.202	57.040	21.904	1.00 39.38	C
MOTA	1137	C	SER	Α	263	57.161	57.641	23.302	1.00 38.48	C
MOTA	1138	0	SER	Α	263	58.107	58.300	23.733	1.00 40.33	0
ATOM	1139	CB	SER	Α	263	56.867	58.121	20.869	1.00 38.57	C
ATOM	1140	OG	SER			55.566	58.644	21.047	1.00 45.09	0
ATOM	1141	N	ASP	Α	264	56.057	57.425	24.005	1.00 35.74	N
MOTA	1142	CA			264	55.913	57.920	25.366	1.00 33.57	С
ATOM	1143	C	ASP			55.358	56.776	26.217	1.00 33.27	С
MOTA	1144	Ō			264	54.144	56.587	26.313	1.00 32.17	. 0
ATOM	1145	СВ			264	54.975	59.136	25.399	1.00 32.37	c
ATOM	1146	CG			264	54.581	59.537	26.812	1.00 32.47	C
ATOM	1147		ASP			55.252	59.113	27.781	1.00 30.31	0
ATOM	1148		ASP			53.598	60.287	26.957	1.00 32.93	ō
ATOM	1149	N			265	56.265	56.014	26.822	1.00 32.50	N
ATOM	1150	CA			265	55.872	54.888	27.649	1.00 32.54	C
ATOM	1151	C			265	55.400	55.262	29.039	1.00 32.31	C
ATOM	1152	0			265	54.959	54.397	29.799	1.00 32.72	. 0
ATOM	1152	N			266	55.502	56.539	29.390	1.00 33.32	N
									1.00 31.81	C
ATOM	1154	CA			266	55.057	56.985	30.705		C
ATOM	1155	C			266	53.540	57.082	30.577	1.00 33.52	0
MOTA	1156	0			266 .	52.967	58.166	30.582	1.00 31.71	
ATOM	1157	CB			266	55.664	58.352	31.043	1.00 30.79	C
MOTA	1158	CG			266	55.742	58.641	32.525	1.00 32.48	C
MOTA	1159		PHE			55.019	57.877	33.450	1.00 31.15	C
ATOM	1160		PHE			56.534	59.690	32.997	1.00 31.72	C
MOTA	1161		PHE			55.085	58.153	34.823	1.00 31.90	C
ATOM	1162		PHE			56.611	59.976	34.361	1.00 31.70	C.
MOTA	1163	CZ			266	55.883	59.206	35.281	1.00 32.01	C
MOTA	1164	N			267	52.896	55.922	30.468	1.00 35.51	N
MOTA	1165	CA			267	51.455	55.859	30.272	1.00 35.95	С
MOTA	1166	C			267	50.735	54.762	31.045	1.00 36.73	С
MOTA	1167	0			267	51.233	53.644	31.187	1.00 34.99	0
MOTA	1168	СВ			267	51.169	55.671	28.785	1.00 36.57	C
ATOM	1169	OG			267	49.795	55.428	28.553	1.00 40.30	0
MOTA	1170	N			268	49.543	55.089	31.523	1.00 37.27	N
MOTA	1171	CA			268	48.736	54.133	32.252	1.00 38.55	C
MOTA	1172	G.	GLU	A	268	48.437	52.945	31.331	1.00 38.48	С
MOTA	1173	0			268	48.204	51.830	31.797	1.00 38.40	, 0
MOTA	1174	CB			268	47.436	54.793	32.719	1.00 39.99	, С
MOTA	1175	CG	GLU	Α	268	46.601	53.903	33.614	1.00 44.01	С
ATOM	1176	CD	GLU	А	268	45.427	54.627	34.254	1:00 46.54	C
MOTA	1177	OE1	GLU	Α	268	44.703	53.969	35.037	1.00 48.88	0
MOTA	1178	OE2	GLU	Α	268	45.230	55.836	33.983	1.00 44.63	0
MOTA	1179	N	TRP	Α	269	48.453	53.184	30.022	1.00 38.21	N
MOTA	1180	CA	TRP	Α	269	48.198	52.114	29.061	1.00 39.86	C
MOTA	1181	C	TRP	А	269	49.267	51.024	29.131	1.00 39.35	C
ATOM	1182	0	TRP	Α	269	48.967	49.849	28.917	1.00 40.08	0
ATOM	1183	CB	TRP	Α	269	48.129	52.657	27.630	1.00 41.72	C
MOTA	1184	CG	TRP	Α	269	46.968	53.561	27.393	1.00 46.52	С
ATOM	1185	CD1	TRP	A	269	47.004	54,914	27.207	1.00 46.39	C
ATOM	1186				269	45.585	53.186	27.347	1.00 47.71	C
MOTA	1187				269	45.731	55.404	27.049	1.00 47.84	N
ATOM	1188				269	44.841	54.366	27.130	1.00 48.66	C
MOTA	1189				269	44.903	51.969	27.470	1.00 49.25	c
ATOM	1190				269	43.445	54.364	27.032	1.00 49.71	· c
MOTA	1191				269	43.513	51.966	27.373	1.00 49.48	С
ATOM	1192				269	42.802	53.158	27.156	1.00 50.26	C
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ATOM	1193	N	GLN	Α	270		50.512	51.401	29.411	1.00 37.64	N
MOTA	1194	CA	GLN				51.575	50.401	29.506	1.00 37.63	С
MOTA	1195	C	GLN				51.402	49.609	30.803	1.00 37.10	C
ATOM	1196	0	GLN				51.661	48.410	30.838	1.00 37.39	0
ATOM	1197	CB	GLN				52.972	51.053	29.461	1.00 35.59	C
ATOM	1198	CG	GLN				53.233	51.888	28.205	1.00 34.03	С
ATOM	1199	CD	GLN				54.518	51.520	27.470	1.00 33.74	C
ATOM	1200		GLN				55.417	50.883	28.024	1.00 31.90	0
ATOM	1201		GLN				54.615	51.943	26.217	1.00 31.81	N
ATOM	1202	N	LYS				50.955	50.276	31.864	1.00 37.76	N
ATOM	1202	CA	LYS				50.737	49.592	33.135	1.00 39.58	C
	1203	C	LYS				49.646	48.532	32.968	1.00 39.28	C
ATOM	1204	0	LYS				49.780	47.412	33.455	1.00 39.33	0
ATOM		CB	LYS				50.320	50.574	34.228	1.00 41.44	C
ATOM	1206						50.086	49.901	35.578	1.00 43.95	Ċ
ATOM	1207	CG	LYS					50.909	36.688	1.00 46.05	C
ATOM	1208	CD	LYS				49.844			1.00 48.90	C
ATOM	1209	CE	LYS				49.756	50.209	38.044	1.00 50.93	N
ATOM	1210	NZ	LYS				49.762	51.161	39.201	1.00 30.93	N
MOTA	1211	N	ILE				48.574	48.896	32.269		C
MOTA	1212	CA	ILE				47.462	47.984	32.029	1.00 39.12	C
MOTA	1213	C	ILE				47.926	46.793	31.198	1.00 39.33	
MOTA	1214	0	ILE				47.616	45.654	31.517	1.00 40.20	0
MOTA	1215	CB			272		46.297	48.701	31.300	1.00 38.48	C
MOTA	1216	CG1					45.626	49.687	32.257	1.00 38.00	C
ATOM	1217	CG2	ILE				45.286	47.682	30.781	1.00 38.67	C
MOTA	1218	CD1	ILE	Α	272		44.609	50.606	31.596	1.00 39.18	С
ATOM	1219	N	THR	Α	273		48.685	47.061	30.143	1.00 38.73	N
ATOM	1220	CA	THR	A	273		49.184	45.999	29.287	1.00 38.01	C
ATOM	1221	С	THR	Α	273		50.089	45.016	30.030	1.00 39.07	C
ATOM	1222	0	THR	Α	273		49.935	43.802	29.896	1.00 38.49	0
ATOM	1223	CB	THR	Α	273		49.959	46.577	28.091	1.00 37.70	С
ATOM	1224	OG1	THR	A	273		49.086	47.409	27.316	1.00 37.99	0
ATOM	1225	CG2	THR	Α	273		50.494	45.458	27.212	1.00 36.21	C
ATOM	1226	N	ILE	Α	274.		51.045	45.537	30.797	1.00 38.89	N
ATOM	1227	CA			274		51.958	44.681	31.547	1.00 38.36	C
MOTA	1228	С			274		51.168	43.894	32.586	1.00 39.27	С
ATOM	1229	0			274		51.452	42.726	32.847	1.00 37.60	0
ATOM	1230	CB			274		53.040	45.507	32.277	1.00 38.10	С
ATOM	1231		ILE				53.911	46.250	31.259	1.00 38.10	C
ATOM	1232		ILE				53.887	44.588	33.163	1.00 37.28	С
ATOM	1233		ILE				54.879	47.247	31.888	1.00 37.22	C
MOTA	1234	N			275		50.177	44.547		1.00 39.95	N
MOTA	1235	CA			275		49.361	43.884	34.183	1.00 41.68	C
MOTA	1236	C			275		48.607	42.702	33.600	1.00 41.85	C
MOTA	1237	Ö			275		48.576	41.622	34.187	1.00 42.65	0
ATOM	1238	N			276		48.002	42.904	32.437	1.00 41.82	N
ATOM	1239	CA			276	٠.		41.847	31.785	1.00 42.57	C
ATOM	1240	C			276		48.144	40.658	31.487	1.00 43.64	С
	1241	0			276		47.707	39.505	31.545	1.00 42.42	0
ATOM ATOM	1241	CB			276		46.641	42.356	30.479	1.00 42.84	Ċ
ATOM		CG			276		45.770	41.356	29.809	1.00 43.77	C
MOTA	1243						44.431	41.168	30.008	1.00 44.10	C
MOTA	1244				276		44.431	40.390	28.829	1.00 44.10	C
MOTA	1245				276			40.390	29.209	1.00 43.95	N
ATOM	1246				276		43.972	39.651	29.209	1.00 43.33	C
MOTA	1247				276		45.018	40.077		1.00 44.37	C
MOTA	1248				276		47.391				C
MOTA	1249	ÇZ2	TRP	Α	276		45.049	38.620	27.533	1.00 44.03	C

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ATOM	1250	CZ3	TRP	Α	276	47.424	39.049	27.278	1.00 44.60	С
ATOM	1251	CH2	TRP	Α	276	46.256	38.333	26.946	1.00 44.88	С
ATOM	1252	N	ILE	Α	277	49.401	40.945	31.159	1.00 43.10	N
ATOM	1253	CA	ILE			50.366	39.899	30.849	1.00 43.16	C
ATOM	1254	C	ILE			50.781	39.127	32.101	1.00 44.32	, C
		0	ILE			50.872	37.901	32.079	1.00 43.89	0
ATOM	1255		ILE			51.619	40.490	30.160	1.00 42.16	С
MOTA	1256	CB						28.759	1.00 40.86	C
ATOM	1257	CG1	ILE			51.249	40.985		1.00 41.70	C
MOTA	1258	CG2	ILE			52.724	39.444	30.084		C
MOTA	1259	CD1	ILE			52.370	41.677	28.027	1.00 39.92	
ATOM	1260	N	AŖĠ	A	278	51.029	39.845	33.190	1.00 45.51	N
MOTA	1261	CA	ARG	Α	278	51.427	39.217	34.445	1.00 47.63	C
ATOM	1262	C	ARG	Α	278	50.313	38.350	35.026	1.00 49.58	С
ATOM	1263	0	ARG	A	278	50.570	37.299	35.617	1.00 49.82	0
MOTA	1264	CB	ARG	Α	278	51.815	40.287	35.466	1.00 46.39	C
MOTA	1265	CG	ARG	A	278	53.125	40.967	35.172	1.00 44.78	С
ATOM	1266	CD	ARG			54.320	40.087	35.522	1.00 43.71	· C
ATOM	1267	NE	ARG			55.551	40.701	35.032	1.00 42.04	. N
	1268	CZ	ARG			56.199	40.311	33.942	1.00 40.35	C
ATOM		NH1	ARG			55.751	39.287	33.229	1.00 38.71	. и
ATOM	1269					57.272	40.976	33.536	1.00 39.83	N
ATOM	1270		ARG					34.853	1.00 51.53	N
MOTA	1271	N	GLU			49.077	38.801			C
MOTA	1272	CA	GLU			47.908	38.094	35.359	1.00 53.86	C
MOTA	1273	С	GLU			47.596	36.819	34.575	1.00 53.60	
ATOM	1274	0	GLU	A	279	47.070	35.854	35.127	1.00 53.73	0
MOTA	1275	CB	GLU	A	279	46.703	39.048	35.343	1.00 56.33	C
ATOM	1276	CG	GLU	Α	279	45.337	38.391	35.440	1.00 61.52	C
ATOM	1277	CD	GLU	Α	279	44.917	37.730	34.137	1.00 64.89	C
MOTA	1278	OE1	GLU	Α	279	44.882	38.429	33.096	1.00 66.72	0
MOTA	1279	OE2	GLU			44.623	36.512	34.154	1.00 66.94	0
MOTA	1280	N			280	47.942	36.813	33.294	1.00 53.24	. N
ATOM	1281	CA			280	47.672	35.671	32.432	1.00 53.14	C
ATOM	1282	C			280	48.863	34.724	32.294	1.00 52.81	C
ATOM	1283	0			280	48.685	33.537	32.029	1.00 52.92	C
					280	47.250	36.182	31.049	1.00 55.15	C
ATOM	1284	CB					35.209	30.199	1.00 57.74	C
ATOM	1285	CG			280	46.435	34.157	29.519	1.00 59.91	
MOTA	1286	CD			280	47.296			1.00 61.61	Ċ
MOTA	1287	CE			280	46.441	33.170	28.715		V.
MOTA	1288	NZ			280	45.645	33.828		1.00 61.74	N.
MOTA	1289	N			281	50.074	35.241	32.490	1.00 51.29	
ATOM		CA				51.273	34.426	32.338	1.00 47.99	C
MOTA	1291	С	TYR	Α	281	52.260	34.496	33.494	1.00 46.98	C
MOTA	1292	0	TYR	Α	281	53.268	33.794	33.485	1.00 46.65	C
MOTA	1293	CB	TYR	Α	281	52.016	34.835	31.066	1.00 47.79	C
ATOM	1294	CG	TYR	Α	281	51.239	34.703	29.778	1.00 46.17	C
MOTA	1295	CD1	TYR	Α	281	51.086	33.465	29.154	1.00 46.76	C
ATOM	1296				281	50.699	35.828	29.153	1.00 45.95	C
ATOM	1297				281	50.420	33.353	27.930	1.00 46.42	. (
ATOM	1298				281	50.032	35.729	27.939	1.00 45.43	(
ATOM	1299	CEZ			281	49.897	34.492	27.330	1.00 46.84	(
						49.255	34.401	26.118	1.00 47.66	Č
ATOM	1300	OH			281			34.484	1.00 46.78	1
ATOM .	1301				282	51.990	35.336		1.00 46.78	(
ATOM	1302	CA			282	52.926	35.458			
MOTA	1303	C			. 282	54.252	35.993			(
MOTA	1304	0			. 282	54.270	36.784		1.00 45.90	1
MOTA	1305	N			283	55.362	35.566	35.660	1.00 49.43	
MOTA	1306	CA	ASP	Α	283	56.682	36.019	35.223	1.00 50.90	(

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MOTA	1307	С	ASP	A	283	57.290	35.115	34.146	1.00 5			С
MOTA	1308	0	ASP	А	283	58.501	35.117	33.940	1.00 5	51.46		0
ATOM	1309	CB	ASP	Α	283	57.637	36.099	36.418	1.00 5	52.54		С
ATOM	1310	CG	ASP	Α	283	57.266	37.208	37.395	1.00 5	6.76		С
ATOM	1311	OD1	ASP			57.213	38.387	36.974	1.00 5	57.47		0
ATOM	1312		ASP			57.034	36.903	38.587	1.00 5	57.67		Ο.
MOTA	1313	N	LYS			56.452	34.354	33.450	1.00 5			N
		CA	LYS			56.935	33.443	32.412	1.00			С
ATOM	1314						34.116	31.052	1.00 4			C
ATOM	1315	С	LYS			57.073		30.168	1.00			0
ATOM	1316	0	LYS			57.780	33.632		1.00			C
ATOM	1317	CB	LYS			56.003	32.229	32.297				
ATOM	1318	CG			284	56.138	31.226	33.449	1.00 5			C
MOTA	1319	CD	LYS	Α	284	55.845	31.868	34.802	1.00			C
MOTA	1320	CE	LYS	А	284	56.104	30.899	35.950	1.00			С
MOTA	1321	NZ	LYS	Α	284	55.874	31.551	37.276	1.00	54.97		N
MOTA	1322	N	VAL	Α	285	56.374	35.227	30.880	1.00 4	46.54		N
ATOM	1323	CA	VAL	Α	285	56.445	35.969	29.634	1.00 4	43.33		С
ATOM	1324	С	VAL	Α	285	57.170	37.270	29.950	1.00	41.39		С
ATOM	1325	0				. 56.759	38.019	30.840	1.00	40.81		0
ATOM	1326	CB			285	55.039	36.252	29.086	1.00	43.01		С
ATOM		. CG1				55.122	37.183	27.887	1.00			С
			VAL			54.380	34.936	28.690	1.00			С
ATOM	1328					58.261	37.520	29.234	1.00			N
ATOM	1329	N			286			29.451	1.00		`	C
ATOM	1330	CA			286	59.060	38.720					C
MOTA	1331	C			286	58.594	39.861	28.556	1.00			
MOTA	1332	0			286	58.383	39.680	27.359	1.00			0
MOTA	1333	CB			286	60.541	38.417	29.193	1.00			C
MOTA	1334	CG	LYS	Α	286	61.077	37.232	29.993	1.00			C
ATOM	1335	CD	LYS	Α	286	60.840	37.401	31.495	1.00			С
ATOM	1336	CE	LYS	Α	286	61.373	36.207	32.282	1.00	35.15		C
ATOM	1337	NZ	LYS	Α	286	61.155	36.341	33.759	1.00	35.87		N
ATOM	1338	N			287	58.437	41.042	29.139	1.00	33.15		N
MOTA	1339	CA			287	57.979	42.185	28.367	1.00	33.28		C
ATOM	1340	С			287	58.706	43.480	28.730.	1.00	32.69		C
MOTA	1341	0			287	58.745	43.886	29.892	1.00	32.80		0
MOTA	1342	CB			287	56.437	42.379	28.543	1.00			C
MOTA	1343				287	56.083	42.447	30.020	1.00			C
					287	55.978		27.843	1.00			C
ATOM	1344					59.295	44.113	27.722	1.00			N
ATOM	1345	N			288	_			1.00			C
ATOM	1346	CA			288	59.983	45.373	27.935				C
ATOM	1347	Ç			288	58.966	46.477	27.731		32.40	•	
ATOM	1348	0			288	57.953	46.263	27.056	1.00			0
MOTA	1349	N			289	59.221	47.646	28.309	1.00			N
MOTA	1350	CA	ALA	A	289	58.309	48.783	28.190	1.00			C
MOTA	1351	C			289	59.088	50.084	27.944	1.00			С
MOTA	1352	0	ALA	A	289	60.304	50.126	28.138	1.00			0
MOTA	1353	CB	ALA	A	289	57.463	48.899	29.464		31.09		C
MOTA	1354	N	GLY	Α	290	58.384	51.135	27.519	1.00	32.95		N
MOTA	1355	CA	GLY	Α	290	59.027	52.415	27.242	1.00	33.02		C
MOTA	1356	C	GLY	Α	290	58.397	53.107	26.039	1.00	33.75		C
ATOM	1357	Ō			290	57.396	52.622	25.517	1.00	34.16		0
ATOM	1358	N			291	58.975	54.210	25.560		32.53		N
	1359	CA			291	60.199	54.804	26.095		31.60		C
ATOM						59.964	55.899	27.134		31.33		C
MOTA	1360	C			291					30.56		0
MOTA	1361	0			. 291	58.936	56.577	27.123				C
MOTA	1362	CB			. 291	61.019	55.405	24.943		30.32		C
MOTA	1363	CG	ASN	A	. 291	61.501	54.354	23.958	1.00	31.30		

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MOTA	1364		ASN			60.981	53.240	23.923		31.67		0
MOTA	1365	ND2	ASN	A	291	62.495	54.708	23.147	1.00	28.26		N
ATOM	1366	N	ILE	Α	292	60.933.	56.052	28.033	1.00	30.09		N
ATOM	1367	CA	ILE	Α	292	60.904	57.090	29.053	1.00	30.04		C
MOTA	1368	С	ILE	A	292	62.276	57.774	29.013	1.00	30.43		С
ATOM	1369	0	ILE			63.205	57.266	28.375		30.27		0
ATOM	1370	СВ	ILE			60.583	56.526	30.484		29.76		C
ATOM	1371	CG1	ILE			61.381	55.253	30.787		30.31		C
ATOM	1372	CG2	ILE			59.105	56.229	30.588		30.24		C
ATOM	1373	CD1	ILE			62.856	55.473	31.028		29.06		C
MOTA	1374	N	VAL			62.409	58.924	29.668		30.29		N
MOTA	1375	CA	VAL			63.680	59.640	29.641		29.96		С
MOTA	1376	C	VAL	Α	293	64.153	60.149	30.991	1.00	30.54		С
MOTA	1377	0	VAL	Α	293	65.175	60.829	31.068	1.00	30.92		0
ATOM	1378	CB	VAL	Α	293	63.612	60.839	28.680	1.00	29.70		С
MOTA	1379	CG1	VAL	Α	293	63.492	60.351	27.238	1.00	27.77		С
ATOM	1380		VAL			62.418	61.717	29.045		28.93		C
MOTA	1381	N	ASP			63.414	59.841	32.053		29.98		N
ATOM	1382	CA	ASP			63.822	60.282	33.384		30.26		C
		C	ASP							29.51		C
MOTA	1383					63.503	59.249	34.465				
ATOM	1384	0	ASP			62.859	58.237	34.201		28.45		0.
MOTA	1385	CB	ASP			63.184	61.645	33.733		29.22		C
MOTA	1386	CG	ASP			61.667	61.579	33.893		30.83		С
MOTA	1387	OD1	ASP	Α	294	61.069	60.517	33.634		30.38		0
MOTA	1388	OD2	ASP	Α	294	61.065	62.609	34.277	1.00	31.14		0
MOTA	1389	N	GLY	Α	295	63.970	59.516	35.680	1.00	30.57		N
MOTA	1390	CA	GLY	A	295	63.739	58.613	36.793	1.00	32.07	•	C
MOTA	1391	С	GLY	A	295	62.278	58.313	37.065	1.00	33.84		С
ATOM	1392	Ο.	GLY			61.928	57.165	37.359		33.24		0
ATOM	1393	N	GLU			61.426	59.337	36.986		35.06		N
ATOM	1394	CA	GLU			59.986	59.172	37.221		36.02		C
ATOM	1395	C	GLU			59.400	58.100	36.315		34.20		C
			GLU									
MOTA	1396	0				58.739	57.179	36.775		34.47		0
ATOM	1397	CB	GLU			59.222	60.473	36.938		39.08		C
MOTA	1398	CG	GLU			59.026	61.420	38.101		44.63		С
ATOM	1399	CD	GLU		,	57.731	62.229	37.955		49.36		C
MOTA	1400	OE1	${\tt GLU}$			57.490	62,820	36.868		49.76		0
MOTA	1401	OE2	GLU	Α	296	56.946	62.266	38.930	1.00	52.97		0
MOTA	1402	N	GLY	Α	297	59.634	58.251	35.015	1.00	34.02		N
MOTA	1403	CA	GLY	Α	297	59.120	57.307	34.040	1.00	32.68		С
MOTA	1404	C	GLY	A	297	59.651	55.901	34.239	1.00	32.72		С
MOTA	1405	0			297	58.912	54.930	34.091		33.28		0
MOTA	1406	N			298	60.937	55.791	34.558		31.86		N
ATOM	1407	CA			298	61.557	54.490	34.793		32.60		C
ATOM	1408	C			298	60.832	53.804	35.946		33.15		C
												0
ATOM	1409	0			298	60.382		35.829		33.25		
ATOM	1410	CB			298	63.029	54.656	35.183		30.95		C
ATOM	1411	CG			298	63.635	53.414	35.773		31.63		С
MOTA	1412		PHE			64.151	52.414	34.953		31.00		С
MOTA	1413	CD2	PHE	A	298	63.622	53.209	37.149	1.00	31.36		C
MOTA	1414	CE1	PHE	Α	298	64.641	51.221	35.498		30.09		С
MOTA	1415	CE2	PHE	A	298	64.108	52.023	37.701	1.00	30.73		С
MOTA	1416	CZ	PHE	A	298	64.616	51.028	36.871		30.06		С
MOTA	1417	N			299		~54.528	37.057		33.22		N
ATOM	1418	CA			299	60.111	54.074	38.291		34.33		C
ATOM	1419	C			299	58.671	53.593	38.074		34.12		C
ATOM	1420	0			299	58.252	52.577	38.635		32.73		0
017	1740	J	מאמ	~	277	20.222	52.511	50.055	1.00	12.13		J

ATOM	1421	CB	ARG	Α	299		60.161	55.228	39.300	1.00			С
MOTA	1422	CG	ARG	A	299		59.224	55.130	40.491	1.00 4			С
MOTA	1423	CD	ARG	Α	299		59.892	54.483	41.682	1.00	42.59		С
ATOM	1424	NE	ARG	Α	299		61.160	55.121	42.041	1.00 4	44.25		N
ATOM	1425	CZ	ARG				61.927	54.709	43.050	1.00 4	44.43		С
ATOM	1426		ARG				61.544	53.677	43.791	1.00 4	42.61		N
ATOM	1427		ARG				63.085	55.304	43.304	1.00	44.39		N
ATOM	1428	N	TYR				57.920	54.318	37.255	1.00	32.22		N
ATOM	1429	CA	TYR				56.540	53.948	36.981	1.00			C
ATOM	1430	C	TYR				56.453	52.607	36.251	1.00			C
ATOM	1431	0	TYR				55.643	51.750	36.606	1.00			0
ATOM	1432	CB	TYR				55.855	55.027	36.143	1.00			C
MOTA	1433	CG	TYR				54.398	54.736	35.864	1.00			С
	1434	CD1					53.418	54.973	36.828	1.00			C
ATOM			TYR				54.002	54.216	34.637	1.00			C
ATOM	1435						52.073	54.700	36.568	1.00			C
ATOM	1436	CE1	TYR				52.670	53.942	34.369	1.00			C
ATOM	1437	CE2	TYR					54.186	35.334		31.71		C
ATOM	1438	CZ ·			300		51.712		35.041	1.00			0
MOTA	1439	OH			300	-	50.396			1.00			N
ATOM	1440	N			301		57.275	52.429	35.222	1.00			C
MOTA	1441	CA			301		57.257	51.180	34.477				C
ATOM	1442	С			301		57.881	50.045	35.304	1.00			0
MOTA	1443	0_			301		57.547	48.878	35.114	1.00			
MOTA	1444	CB			301		57.992	51.349	33.140	1.00			C
ATOM	1445	CG			301		57.342	52.341	32.160	1.00			C
MOTA	1446		LEU				58.174	52.459	30.891	1.00			
MOTA	1447	CD2	LEU				55.928	51.870	31.823	1.00			C
MOTA	1448	N			302		58.780	50.390	36.220	1.00			N
MOTA	1449	CA			302		59.418	49.385	37.066	1.00			C
ATOM	1450	С	ALA	Α	302		58.355	48.806	38.008	1.00			. C
ATOM	1451	0	ALA	A	302		58.169	47.590	38.082		34.00	ť	0
MOTA	1452	CB			302		60.563	50.012	37.866		31.06		C
MOTA	1453	N	ASP	A	303		57.652	49.686	38.711		34.91		N
MOTA	1454	CA	ASP	A	303		56.595	49.262	39.618		35.64		C
MOTA	1455	C	ASP	Α	303		55.485	48.552	38.846		36.85		С
MOTA	1456	0	ASP	A	303		54.761	47.737	39.408		37.85		0
MOTA	1457	CB	ASP	Α	303		56.008	50.458	40.365		35.88		C
MOTA	1458	CG	ASP	Α	303		56.956	51.022	41.398		38.13		C
MOTA	1459	OD1	ASP	Α	- 303		57.843	50.276	41.863		40.12		0
MOTA	1460	OD2	ASP	A	303		56.800	52.205		1.00	40.53		0
MOTA	1461	N	ALA	Α	304		55.356	48.859	37.557	1.00	36.62		N
ATOM	1462	CA	ALA	A	304		54.331	48.233	36.725		36.26		C
MOTA	1463	C	ALA	A	304		54.719	46.802	36.343	1.00	36.18		C
MOTA	1464	0	ALA	A	304		53.876	46.035	35.868	1.00	35.97		0
ATOM	1465	CB	ALA	A	304		54.095	49.063	35.466	1.00	35.66		C
ATOM	1466	N	GLY	Α	305		55.994	46.454	36.519	1.00	35.62		N
ATOM	1467	CA	GLY	Α	305		56.440	45.102	36.212	1.00	33.54		С
ATOM	1468	С			305		57.266	44.840	34.964	1.00	34.83		C
MOTA	1469	0			305		57.559	43.678	34.654	1.00	34.47		0
ATOM	1470	N			306		57.648	45.890	34.239	1.00	34.51		N
ATOM	1471	CA			306			45.718	33.022	1.00	34.01		C
ATOM	1472	C			306		59.718	44.902	33.304	1.00	33.98		C
ATOM	1473	Ö			306	~	60.302	45.017	34.378		33.26		0
ATOM	1474	CB			306		58.825	47.084	32.450		33.19		C
ATOM	1475	N			307		60.137				34.27		N
ATOM	1476	CA			307		61.341				35.04		C
MOTA	1477	C			307		62.605				34.78		С
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MOTA	1478	0	ASP	Α	307	63.716	43.658	32.462	1.00 35.12	0
MOTA	1479	CB	ASP	Α	307	61.191	41.967	31.684	1.00 34.06	C
MOTA	1480	CG	ASP	Α	307	60.205	41.010	32.322	1.00 35.84	C
MOTA	1481	OD1	ASP	Α	307	60.511	40.519	33.429	1.00 33.94	0
MOTA	1482	OD2	ASP	Α	307	59.127	40.764	31.733	1.00 35.52	0
ATOM	1483	N	PHE			62.418	45.042	31.255	1.00 33.72	N
ATOM	1484	CA	PHE			63.499	45.920	30.838	1.00 32.62	С
ATOM	1485	C	PHE			62.811	47.210	30.396	1.00 32.76	C
ATOM	1486	0	PHE			61.660	47.194	29.961	1.00 32.31	0
ATOM	1487	CB	PHE			64.389	45.282	29.751	1.00 30.88	C
ATOM	1488	CG	PHE			63.833	45.325	28.351	1.00 31.29	C
ATOM	1489		PHE			63.823	46.514	27.622	1.00 30.95	C
ATOM	1490		PHE			63.399	44.152	27.729	1.00 31.69	C
ATOM	1491		PHE			63.396	46.536	26.289	1.00 31.24	C
ATOM	1492	CE2	PHE			62.968	44.158	26.393	1.00 32.80	С
ATOM	1493	CZ	PHE			62.968	45.356	25.671	1.00 33.19	С
ATOM	1494	N	ILE			63.499	48.330	30.558	1.00 32.53	N
	1495	CA	ILE			62.919	49.618	30.221	1.00 31.47	С
MOTA		C	ILE			63.723	50.323	29.138	1.00 31.48	C
ATOM	1496	0	ILE			64.952	50.428	29.228	1.00 29.64	. 0
ATOM	1497	CB	ILE			62.809	50.477	31.502	1.00 31.63	C
MOTA	1498		ILE			61.767	49.835	32.431	1.00 29.83	c
ATOM	1499	CG1 CG2	ILE			62.467	51.924	31.160	1.00 30.76	Ċ
ATOM	1500					61.696	50.434	33.823	1.00 30.70	C
MOTA	1501	CD1	ILE			63.016	50.794	28.109	1.00 30.52	N
MOTA	1502	N	LYS			63.649	51.456	26.977	1.00 30.32	C
ATOM	1503	CA	LYS				52.975	27.166	1.00 30.46	c
ATOM	1504	C	LYS			63.730			1.00 30.40	0
ATOM	1505	0	LYS			62.746	53.630	27.515	1.00 30.84	C
ATOM	1506	CB	LYS			62.899	51.092	25.693		C
MOTA	1507	CG	LYS			63.787	50.985	24.461	1.00 30.94 1.00 29.84	C
MOTA	1508	CD	LYS			63.396	49.797	23.572		. c
MOTA	1509	CE			310	62.017	49.979	22.964	1.00 28.94	И
ATOM	1510	NZ			310	61.928	51.268	22.219	1.00 28.29	N
MOTA	1511	N			311	64.917	53.517	26.920	1.00 29.41	C
MOTA	1512	CA			311	65.197	54.943	27.097	1.00 29.44	
MOTA	1513	С			311	65.362	55.711	25.796	1.00 29.18	C
MOTA	1514	0			311	66.100	55.288	24.908	1.00 28.56	0
MOTA	1515	CB			311	66.517	55.158	27.887	1.00 28.45	C
MOTA	1516	CG1			311	66.498	54.353	29.186	1.00 27.16	C
MOTA	1517		ILE			66.721	56.653	28.178	1.00 25.82	C
MOTA	1518		ILE			67,864	54.280	29.857	1.00 27.18	C
MOTA	1519	N			312	64.690	56.852	25.692	1.00 30.57	N
MOTA	1520	ĊA			312		57.660	24.502	1.00 30.97	C
MOTA	1521	С			312	63.637	58.202	23.798	1.00 33.02	C
MOTA	1522	0			312	62.739	57.460	23.412	1.00 32.51	0
MOTA	1523	N			313		59.519	23.631	1.00 35.45	N
MOTA	1524	CA			313	62.558	60.210	22.920	1.00 37.38	C
MOTA	1525	С			313	63.194	61.380	22.181	1.00 40.19	C
MOTA.	1526	0			313	63.759	62.280	22.807	1.00 39.32	0
MOTA	1527	CB			313	61.484	60.766	23.865	1.00 36.69	C
MOTA	1528	CG1	ILE	Α	313	60.825	59.625	24.646	1.00 37.09	C
MOTA	1529	CG2	ILE	A	313	60.437	61.517	23.053	1.00 36.17	C
ATOM	1530	CD1	ILE	Α	313	59.810	60.097	25.666	1.00 34.32	С
ATOM	1531	N	GLY	Α	314	63.121	61.350	20.853	1.00 43.35	N
MOTA	1532	CA	GLY	A	314	63.682	62.424	20.055	1.00 47.92	С
MOTA	1533	C	GLY	A	314	65.013	62.127	19.386	1.00 51.41	С
MOTA	1534	0	GLY	A	314	65.318	62.690	18.333	1.00 52.28	0

MOTA	1535	N	GLY	Α	315	65.804	61.244	19.990	1.00	53.66		N
MOTA	1536	CA	GLY	Α	315	67.109	60.902	19.443	1.00	55.96		С
MOTA	1537	С	GLY			67.151	60.218	18.085	1.00	57.72		С
ATOM	1538	0	GLY			68.050	60.499	17.288		58.05		0
ATOM	1539	N	GLY			66.202	59,320	17.818		58.68		N
ATOM	1540	CA			316	66.174	58.615	16.542		60.38		C
MOTA	1541	C			316	66.578	59.446	15.330		61.63		C
ATOM	1542	0			316		60.617	15.216		61.39		0
						66.212					•	
ATOM	1543	N			317	67.328	58.838	14.415		63.21		N
ATOM	1544	CA			317	67.786	59.529	13.211		64.85		C
ATOM	1545	C			317	66.626	59.987	12.331		66.57		C
ATOM	1546	0			317	66.711	61.022	11.667		66.58		0
MOTA	1547	CB			317	68.714	58.621	12.395		64.42		С
MOTA	1548	OG	SER	Α	317	68.001	57.556	11.787	1.00	62.55		0
MOTA	1549	N	ILE	А	318	65.547	59.212	12.324	1.00	68.56		N
MOTA	1550	CA	ILĖ	Α	318	64.376	59.542	11.517	1.00	71.22		С
MOTA	1551	C	ILE	A	318	63.259	60.192	12.327	1.00	72.91	•	С
ATOM	1552	0	ILE	A	318 .	62.098	60.185	11.913	1.00	73.31		0
MOTA	1553	CB	ILE	Α	318	63.815	58.286	10.805	1.00	71.18		С
MOTA	1554		ILE			63.983	57.051	11.698		71.48		C
ATOM	1555	CG2				64.529	58.080	9.475		70.96		Ċ
MOTA	1556	CD1	ILE			63.326	57.162	13.049		70.32		C
ATOM	1557	N			319	63.617	60.755	13.478		75.09		И
					319							C
MOTA	1558	CA				62.651	61.417	14.350		77.73		
ATOM	1559	C			319	62.958	62.911	14.448		78.61		C
MOTA	1560	0			319	64.091	63.300	14.731		78.56		0
MOTA	1561	СВ			319	62.686	60.789	15.746		78.48		C
MOTA	1562	SG			319	61.465	61.464	16.899		81.82		S
ATOM	1563	N			320	61.947	63.743	14.214		79.90		N
MOTA	1564	CA	ILE	Α	320	62.123	65.194	14.271	1.00	81.47		С
ATOM	1565	C	ILE	Α	320	61.255	65.828	15.362	1.00	82.10		C
MOTA	1566	0	ILE	A	320	60.147	66.298	15.096	1.00	82.35		0
ATOM	1567	CB	ILE	Α	320	61.776	65.850	12.911	1.00	81.84		С
MOTA	1568	CG1	ILE	Α	320	62.556	65.162	11.787	1.00	82.02		С
ATOM	1569	CG2	ILE	Α	320	62.121	67.340	12.946	1.00	82.15		С
MOTA	1570	CD1	ILE	Α	320	62.212	65.669	10.396	1.00	82.11		С
ATOM	1571	N			321	61.775	65.841	16.587		82.35		N
ATOM	1572	CA			321	61.072	66.403	17.738		82.60		C
ATOM	1573	C			321	60.461	67.782	17.469		82.30		C
ATOM	1574	Ö	THR			59.253	67.975	17.619		81.76		Ö
ATOM	1575	CB.			321	62.019	66.527	18.949		82.94		C
ATOM	1576		THR			62.607	65.250	19.232		83.54		0
ATOM	1577		THR			61.257	67.016	20.167		82.53		C
MOTA	1578	N			322	61.306	68.735	17.083		82.27		N
ATOM	1579	CA			322	60.863	70.099	16.800		82.39		C
MOTA	1580	C			322	59.651	70.172	15.878		81.93		С
ATOM	1581	0			322	58.611	70.714	16.254		81.88		0
MOTA	1582	CB	ARG			62.005	70.915	16.191		83.09		C
MOTA	1583	CG	ARG	A	322	63.009	71.456	17.199	1.00	83.95		C
ATOM	1584	CD	ARG	A	322	63.963	72.423	16.516	1.00	84.72		С
ATOM	1585	NE	ARG	A	322	64.729	73.227	17.464	1.00	85.49		N
MOTA	1586	CZ	ARG	Α	322	65.543	74.218	17.108	1.00	85.83		С
ATOM	1587	NH1	ARG	Α	322	65.696	74.526	15.824	1.00	85.76		N
MOTA	1588		ARG			66.203	74.903	18.032		85.80		N
ATOM	1589	N			323	59.791	69.634	14.668		81.06		N
MOTA	1590	CA			323	58.699	69.643	13.697		80.15		С
ATOM	1591	C			323	57.547	68.739	14.131		78.66		C
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ATOM	1592	0	GLU	Α	323	56.713	68.343	13.313	1.00	78.92		0
ATOM	1593	CB	GLU	Α	323	59.205	69.192	12.324	1.00	81.16		C
MOTA	1594	CG	GLU	Α	323	60.194	70.145	11.677	1.00	83.13		C
MOTA	1595	CD	GLU	Α	323	60°.632	69.676	10.302	1.00	84.05		C
MOTA	1596	OE1	GLU	Α	323	61.266	68.602	10.212	1.00	84.52		O.
MOTA	1597	OE2	GLU			60.337	70.381	9.312	1.00	84.85		0
MOTA	1598	N			324	57.500	68.420	15.421		76.17		N
ATOM	1599	CA			324	56.451	67.559	15.947	1.00	73.65		С
MOTA	1600	С			324	55.768	68.105	17.202	1.00	70.58		С
MOTA	1601	0			324	55.066	69.117	17.147		70.75		0
ATOM	1602	CB			324	57.019	66.160	16.218		76.03		C
MOTA	1603	CG			324	57.091	65.267	14.980		78,70		C
MOTA	1604	CD			324	58.247	64.274	15.029		80.71		С
ATOM	1605	OE1	GLN			58.488	63.623	16.050	1.00	81.60		0
MOTA	1606		GLN			58.964	64.150	13.913		81.50		N
ATOM	1607	N			325	55.987	67.439	18.331		66.07		N
ATOM	1608	CA			325	55.358	67.823	19.588		61.45		C
MOTA	1609	С	LYS			56.260	68.589	20.549		57.60		C
MOTA	1610	0	LYS			55.778	69.239	21.479		56.87	*	0
ATOM	1611	CB	LYS			54.817	66.566	20.274		62.25		C
MOTA	1612	CG	LYS			 53.832	65.795	19.402		63.17		C
ATOM	1613	CD	LYS			53.889	64.295	19.660		63.20		C
ATOM	1614	CE			325	53.295	63.928	20.999		62.14		C
ATOM	1615	NZ			325	51.844	64.232	21.055		62.08		N
ATOM	1616	N			326	57.566	68.515	20.335		52.89		N
ATOM	1617	CA			326	58.468	69.220	21.222		48.72		C
ATOM	1618	C			326	58.716	68.493	22.534		45.75		C
ATOM	1619	0	GLY			58.952	69.129	23.557		44.02		0
ATOM	1620	N			327	58.639	67.164	22.510		42.92		N
MOTA	1621	CA			327	58.901	66.362	23.698		41.83		C
ATOM	1622	C			327	60.222	65.632	23.463		40.05		C
ATOM	1623	0			327	60.573	65.316	22.329		39.48		0
ATOM	1624	CB			327	57.777	65.310	23.974		42.64	•	C
ATOM	1625	CG1			327	57.577	64.408	22.754		44.04		C
MOTA	1626	CG2					66.012			44.04		C
MOTA	1627	CD1	ILE		327	56.470 56.582	63.261	24.333		46.03		.C
ATOM							65.374	22.982 24.528		38.80		
ATOM	1628 1629	N CA			328 328	60.964				37.90		N
		CA				62.223	64.681	24.360				C
ATOM ATOM	1630 1631	0	GLY		328	63.289	65.133 65.973	25.334 26.206		36.87 35.37		C 0
			ARG			63.041						-
MOTA	1632 1633	N CA				64.484	64.573	25.175 26.042		34.44		N
ATOM .			ARG			65.602	64.901			32.91		C
ATOM	1634	C	ARG			66.872	64.373	25.389		32.38		C
ATOM	1635	0			329	66.826	63.365	24.689		32.32		0
MOTA	1636	CB			329	65.395	64.239	27.410		32.23		C
ATOM	1637	CG			329	66.233	64.822	28.530		31.22		C
MOTA	1638	CD			329	66.062	64.023	29.813		31.90		C
MOTA	1639	NE	ARG			66.413	64.807	30.991		30.70		N
ATOM	1640	CZ			329	66.373	64.344	32.235		33.01		C
ATOM	1641		ARG			66.002	63.093	32.469		32.08		N
ATOM	1642		ARG			66.692	65.139	33.249		32.28		N
ATOM	1643	N			330	67.999	65.058	25.592		31.61		N
ATOM	1644	CA			330	69.245	64.582	25.012		29.56		C
MOTA	1645	C			330	69.431	63.148	25.481		29.63		. C
ATOM	1646	0			330	69.267	62.861	26.666		29.00		0
ATOM	1647	N			331	69.775	62.253	24.563		29.35		N
MOTA	1648	CA	GLN	A	331	69.936	60.839	24.880	T.00	29.79		C

					,							
MOTA	1649	C	GLN	Α	331	70.913	60.538	26.021	1.00	30.69		C
MOTA	1650	0	GLN	A	331	70.644	59.654	26.840	1.00	30.62		0
ATOM	1651	CB	GLN	Α	331	70.348	60.057	23.625	1.00	29.75		С
ATOM	1652	CG	GLN			70.254	58.531	23.781	1.00	31.50	•	С
ATOM	1653	CD	GLN			68.822	58.039	23.959		33.75		С
ATOM	1654	OE1	GLN			68.590	56.903	24.387		35.72		0
ATOM	1655	NE2	GLN			67.858	58.885	23.623		30.84		N
ATOM	1656	N	ALA			72.039	61.254	26.078		28.60		N
										29.13		C
ATOM	1657	CA	ALA			73.017	61.020	27.142				
ATOM	1658	C	ALA			72.422	61.330	28.513		28.73		C
ATOM	1659	0	ALA			72.495	60.513	29.437		28.92		0
ATOM	1660	CB	ALA			74.281	61.873	26.912		29.21		С
MOTA	1661	N	THR			71.833	62.513	28.639		26.69		N
MOTA	1662	CA	THR			71.229	62.933	29.893		27.66		C
ATOM	1663	C .	THR	A	333	70.126	61.968	30.321	1.00	27.96		C
MOTA	1664	0	THR	Α	333	70.017	61.619	31.496	1.00	27.38		0
MOTA	1665	CB	THR	A	333	70.643	64.347	29.770	1.00	28.02		C
MOTA	1666	OG1	THR	Α	333	71.681	65.249	29.359	1.00	27.47		0
ATOM	1667	CG2	THR	Α	333	70.066	64.804	31.121	1.00	28.00		С
	1668	N	ALA	Α	334	69.317	61.534	29.361	1.00	27.55	-	N
MOŢA	1669	CA	ALA			68.236	60.596	29.642		27.85		С
ATOM	1670	C	ALA			68.795	59.294	30.219		27.98		С
ATOM	1671	Ō	ALA			68.318	58.792	31.238		28.76		Ō
ATOM	1672	CB	ALA			67.448	60.309	28.362		26.67		C
ATOM	1673	N .	VAL			69.809	58.745	29.562		29.11		N
ATOM	1674	CA	VAL			70.416	57.499	30.011		29.37		C
ATOM		C	VAL				57.652			29.55		C
	1675					71.009		31.411				
ATOM	1676	0	VAL			70.721	56.856	32.311		28.49		0
ATOM	1677	CB	VAL			71.524	57.039	29.033		30.52		C
ATOM	1678		VAL			72.291	55.859	29.622		31.70		C
ATOM	1679		VAL			70.904	56.644	27.701		30.54		C
MOTA	1680	N			336	71.823	58.686	31.592		29.23		N
MOTA	1681	CA	ILE			72.464	58.938	32.878	1.00	28.94		С
ATOM	1682	C	ILE	A	336	71.450	59.063	34.013	1.00	30.36		C
MOTA	1683	0	ILE	Α	336	71.652	58.525	35.109	1.00	28.57		0
MOTA	1684	CB	ILE	А	336	73.325	60.216	32.813	1.00	28.69		C
MOTA	1685	CG1	ILE	Α	336	74.531	59.974	31.898	1.00	27.72		C
MOTA	1686	CG2	ILE	Α	336	73.768	60.630	34.211	1.00	24.85		C
MOTA	1687	CD1	ILE	A	336	75.352	61.229	31.609	1.00	29.74		C
MOTA	1688	Ν.	ASP	Α	337	70.351	59.761	33.743	1.00	30.78		N
ATOM	1689	CA	ASP			69.312	59.964	34.746		30.67		С
	1690	C	ASP		*	68.563	58.662	35.065		30.77		C
ATOM	1691	0			337	68.358	58.320	36.229		29.22		Ō
ATOM	1692	СВ	ASP			68.325	61.018	34.250		33.77		Č
ATOM	1693	CG			337	67.287	61.373	35.285		35.46		C
ATOM	1694		ASP				61.806	34.897		36.96		0
						66.180	61.228			38.65		
MOTA	1695		ASP			67.581		36.488				0
ATOM	1696	N	VAL			68.152	57.941	34.027		30.12		N
MOTA	1697	CA			338	67.427	56.693	34.217		29.17		C
ATOM	1698	C	VAL			68.289	55.663	34.935		30.19		C
MOTA	1699	0	VAL			67.808	54.963	35.829		29.30		0
ATOM	1700	CB	VAL			66.947	56.103	32.865		29.20		С
MOTA	1701		VAL			66.423	54.683	33.068		26.29		C
ATOM	1702	CG2	VAL	Α	338	65.845	56.986	32.277	1.00	27.28		С
ATOM	1703	N	VAL			69.556	55.572	34.535	1.00	28.08		N
MOTA	1704	CA	VAL	A	339	70.489	54.636	35.147	1.00	29.13		C
MOTA	1705	C	VAL			70.653	54.889	36.648	1.00	30.51		C

	1700	^	7 7 N T	70	220		70.731	53.943	37.432	1.00 31.60		0
MOTA	1706		VAL							1.00 29.06		C
MOTA	1707		VAL				71.874	54.710	34.457			C
MOTA	1708	CG1					72.931	54.010	35.302	1.00 27.64		
MOTA	1709	CG2	VAL	Α	339		71.789	54.062	33.070	1.00 27.50		C
ATOM	1710	N	ALA	Α	340		70.708	56.158	37.048	1.00 30.84	•	N
ATOM	1711	CA	ALA	Α	340		70.851	56.490	38.463	1.00 31.17		С
MOTA	1712	C	ALA	Α	340		69.610	56.014	39.211	1.00 31.63		C
ATOM	1713		ALA				69.701	55.469	40.313	1.00 32.08		0
ATOM	1714		ALA				71.028	57.999	38.644	1.00 30.25		C
	1715	N	GLU				68.448	56.215	38.601	1.00 31.19		N
ATOM			GLU				67.196	55.810	39.225	1.00 31.45		C
ATOM	1716	CA					67.138	54.290	39.301	1.00 31.09		C
ATOM	1717	C	GLU						40.305	1.00 30.16		ō
ATOM	1718	0	GLU				66.702	53.730		1.00 30.10		C
MOTA	1719	CB	GLU				66.006	56.334	38.419			C
ATOM	1720	CG	GLU				64.668	56.257	39.149	1.00 34.04		
MOTA	1721	CD	GLU	А	341		64.611	57.1 <b>77</b>	40.362	1.00 37.16		C
ATOM	1722	OE1	GLU	Α	341		65.211	58.273	40.313	1.00 38.31		0
MOTA	1723	OE2	GLU	Α	341		63.954	56.816	41.358	1.00 37.63		0
ATOM	1724	N	ARG	A	342		67.578	53:634	38.232	1.00 30.40		N
ATOM	1725	CA	ARG	Α	342		67.585	52.177	38.170	1.00 31.42		C
ATOM	1726	С	ARG				68.469	51.616	39.286	1.00 31.57		C
ATOM	1727	Ō	ARG				68.099	50.646	39.937	1.00 32.09		0
MOTA	1728	СВ	ARG				68.086	51.709	36.791	1.00 31.10		C
		CG			342		68.037	50.192	36.542	1.00 28.82		С
ATOM	1729						69.284	49.477	37.069	1.00 28.26		C
ATOM	1730	CD			342				36.441	1.00 26.03		N
ATOM	1731	NE			342		70.531	49.919				C
MOTA	1732	CZ			342		70.871	49.696	35.172	1.00 26.57		
ATOM	1733		ARG				70.060	49.035	34.360	1.00 25.10		N
MOTA	1734	NH2	ARG				72.043	50.120	34.714	1.00 26.92		N
MOTA	1735	N ·	ASN	Α	343		69.626	52.236	39.508	1.00 31.96		N
MOTA	1736	CA	ASN	Α	343		70.537	51.788	40.557	1.00 33.03		C
ATOM	1737	Ç	ASN	Α	343	•	69.943	52.031	41.946	1.00 34.72		C
MOTA	1738	Ó	ASN	Α	343		70.122	51.220	42.854	1.00 35.11		0
MOTA	1739	CB	ASN	Α	343		71.898	52.478	40.418	1.00 31.35		C
ATOM	1740	CG			343		72.651	52.020	39.176	1.00 32.01		C
ATOM	1741		ASN				72.335	50.976	38.604	1.00 31.68		0
ATOM	1742		ASN				73.657	52.786	38.765	1.00 29.30		N
	1743	N			.344		69.229	53.141		1.00 36.02		N
MOTA					344	• •	68.587	53.446	43.378	1.00 38.22		C
MOTA	1744	CA			•		67.512	52.384	43.615	1.00 37.85		C
ATOM	1745	C			344			51.834	44.709	1.00 37.03		ō
MOTA	1746	0			344		67.392		43.338	1.00 35.02		Ċ
MOTA	1747	CB			344		67.942	54.837				C
ATOM	1748	CG			344		67.139	55.177	44.589	1.00 46.89		
MOTA	1749	CD			344		66.252	56.412	44.393	1.00 51.33		C
MOTA	1750	CE	LYS	A	344		67.040	57.709	44.454	1.00 54.56		C
MOTA	1751	NZ	LYS	A	344		67.416	58.052	45.862	1.00 58.14		N
MOTA	1752	N	TYR	Α	345		66.744	52.092	42.573	1.00 37.18		N
MOTA	1753	CA	TYR	A	345		65.679	51.098	42.639	1.00 36.37		С
MOTA	1754	С	TYR	A	345		66.223	49.722	43.031	1.00 37.15		C
ATOM	1755	0			345		65.615	49.009	43.827	1.00 36.61		0
ATOM	1756	СВ			345		64.987	50.991	41.287	1.00 35.78		C
ATOM	1757	CG			345		63.677	50.235	41.321	1.00 37.12		С
ATOM	1758				345		62.506	50.863	41.736	1.00 36.58		С
					345		63.600	48.905	40.906	1.00 35.92		C
ATOM	1759						61.294	50.196	41.731	1.00 37.36		C
MOTA	1760				345			48.223	40.897	1.00 37.19		C
ATOM	1761				345		62.385			1.00 37.13		C
MOTA	1762	CZ	TYR	. A	345		61.238	48.880	41.309	1.00 37.67		C

MOTA	1763	OH	TYR	Α	345	60.025	48.240	41.280	1.00 3	9.76			0
MOTA	1764	N	PHE	А	346	67.359	49.346	42.452	1.00 3	7.41			N
MOTA	1765	CA	PHE	A	346	67.986	48.064	42.759	1.00 3	8.71			С
MOTA	1766	С	PHE	Α	346	68.354	47.996	44.244	1.00 3	9.07			С
MOTA	1767	0	PHE	A	346	68.162	46.969	44.889	1.00 3	8.25			0
MOTA	1768	CB	PHE	Α	346	69.251	47.869	41.915	1.00 3	7.92			С
MOTA	1769	CG	PHE	Α	346	70.018	46.621	42.252	1.00 3	9.35			С
ATOM	1770	CD1	PHE			69.484	45.362	41.984	1.00 3	8.94			С
MOTA	1771	CD2	PHE			71.277	46.703	42.841	1.00 4				С
ATOM	1772	CE1	PHE			70.190	44.203	42.294	1.00 3	9.83			С
ATOM	1773	CE2	PHE			71.997	45.545	43.159	1.00 4				C
MOTA	1774	CZ	PHE			71.449	44.292	42.883	1.00 4				C
MOTA	1775	N	GLU			68.877	49.096	44.778	1.00 4				N
MOTA	1776	CA	GLU			69.269	49.150	46.183	1.00 4				С
MOTA.	1777	С	GLU			68.091	49.066	47.147	1.00 4				Ċ
MOTA	1778	0	GLU			68.227	48.534	48.249	1.00 4				0
MOTA	1779	СВ	GLU			70.061	50.429	46.472	1.00 4				C
ATOM	1780	CG	GLU			71.410	50.480	45.778	1.00 5				C
ATOM	1781	CD.			347	72.321	49.322	46.176	1.00 5				Ç
ATOM	1782		GLU			73.405	49.177	45.565	1.00 5				0
ATOM	1783		GLU			71.961	48.556	47.101	1.00 5				0
ATOM	1784	N	GLU			66.940	49.582	46.731	1.00 4				N
ATOM	1785	CA	GLU					47.580					
ATOM	1786	C.	GLU			65.760	49.574		1.00 4				C
						64.987	48.265	47.522	1.00 4				C
MOTA	1787	0	GLU			64.437	47.821	48.526	1.00 4				0
ATOM	1788	CB	GLU			64.800	50.705	47.178	1.00 4				C
MOTA	1789	CG	GLU			65.481	52.020	46.833	1.00 4				C
ATOM	1790	CD	GLU			64.505	53.097	46.375	1.00 4				C
MOTA	1791	OE1	GLU			63.565	52.781	45.611	1.00 4				0
ATOM	1792	OE2	GLU			64.694	54.268	46.773	1.00 5				0
MOTA	1793	N	THR			64.954	47.645	46.349	1.00 4				N
MOTA	1794	CA	THR			64.171	46.432	46.159	1.00 3				С
ATOM	1795	С	THR			64.910	45.133	45.859	1.00 3				C
MOTA	1796	0	THR			64.306	44.062	45.895	1.00 3	7.84			0
MOTA	1797	CB	THR			63.173	46.639	45.020	1.00 3				С
MOTA	1798	OG1	THR			63.894	46.724	43.784	1.00 3	37.27			0
ATOM	1799	CG2	THR			62.387	47.933	45.223	1.00 3				C
MOTA	1800	N	GLY	А	350	66.197	45.216	45.550	1.00 3	7.03			N
ATOM	1801	CA	GLY	А	350	66.940	44.014	45.215	1.00 3	6.78			С
MOTA	1802	C	GLY			66.646	43.568	43.787	1.00 3	6.94			С
MOTA	1803	0	GLY	А	350	67.115	42.520	43.340	1.00 3	37.38			0
MOTA	1804	N	ILE			65.863	44.362	43.061	1.00 3	4.88			N
ATOM	1805	CA	ILE	А	351	65.515	44.027	41.683	1.00 3	3.79			C
MOTA	1806	C	ILE	Α	351	66.368	44.835	40.708	1.00 3	32.41			С
ATOM	1807	0	ILE	A	.351	66.378	46.061	40.765	1.00 3	1.22			0
MOTA	1808	CB	ILE	A	351	64.043	44.357	41.381	1.00 3	6.04			С
MOTA	1809	CG1	ILE	А	351	63.125	43.668	42.391	1.00 3	6.61	•		С
MOTA	1810	CG2	ILE	Α	351	63.706	43.948	39.948	1.00 3	5.73			С
MOTA	1811	CD1	ILE	A	351	61.686	44.165	42.331	1.00 3	7.65			С
MOTA	1812	N	TYR			67.078	44.153	39.817	1.00 3				N
MOTA	1813	CA			352	67.904	44.843	38.835	1.00 3				С
ATOM	1814	С	TYR			67.177	44.844	37.493	1.00 3				C
MOTA	1815	0	TYR			66.953	43.791	36.904	1.00 3				ō
ATOM	1816	CB	TYR			69.264	44.158	38.666	1.00 3				C
ATOM	1817	CG	TYR			70.174	44.889	37.695	1.00 3				C
ATOM	1818		TYR			70.998	45.930	38.128	1.00 2				C
MOTA	1819		TYR			70.171	44.575	36.336	1.00 3				C
			- 4.1				22.0,0	20.000	2.00				_

MOTA	1820	CE1	TYR	A	352	71.794	46.638	37.237	1.00 28.10		С
ATOM	1821	CE2	TYR	A	352	70.966	45.280	35.434	1.00 30.54		C
ATOM	1822	CZ	TYR	A	352	71.775	46.309	35.895	1.00 29.18		С
MOTA	1823	OH	TYR	A	352	72.580	46.996	35.019	1.00 31.65		0
ATOM	1824	N	ILE	A	353	66.811	46.027	37.010	1.00 32.84		N
ATOM	1825	CA	ILE	Α	353	66.113	46.119	35.735	1.00 31.85		C
ATOM	1826	C.	ILE	Α	353	67.028	46.626	34.634	1.00 31.84		С
ATOM	1827	0	ILE	Α	353	67.506	47.760	34.679	1.00 32.46		0
ATOM	1828	CB	ILE	Α	353	64.900	47.048	35.835	1.00 32.61		С
ATOM	1829	CG1	ILE			63.962	46.536	36.936	1.00 34.08		С
ATOM	1830		ILE			64.181	47.105	34.487	1.00 33.22		С
ATOM	1831		ILE			62.793	47.431	37.244	1.00 32.45		С
ATOM	1832	N	PRO			67.303	45.779	33.634	1.00 30.90		N
ATOM	1833	CA	PRO			68.177	46.197	32.533	1.00 29.68		С
ATOM	1834	C	PRO			67.528	47.344	31.763	1.00 29.05	J	C
ATOM	1835	Ō	PRO			66.308	47.368	31.600	1.00 28.14	-	0
ATOM	1836	СВ	PRO			68.293	44.934	31.679	1.00 28.34		C
ATOM	1837	CG	PRO			68.051	43.808	32.680	1.00 29.10		C
ATOM	1838	CD	PRO			66.921	44.360	33.506	1.00 29.33		C
ATOM	1839	N	VAL			68.330	48.302	31.301	1.00 28.33		N
ATOM	1840	CA			355	67.771	49.404	30.529	1.00 27.79		C
		CA	VAL				49.446	29.151	1.00 27.79		C
MOTA	1841				355	68.406		28.958	1.00 27.30		0
ATOM	1842	O				69.552 67.931	49.044 50.788		1.00 28.70		C
ATOM	1843	CB	VAL					31.246			
ATOM	1844		VAL			67.191	50.759	32.584	1.00 27.11		C
ATOM	1845		VAL			69.406	51.147	31.427	1.00 24.91		C
ATOM	1846	N			356	67.640	49.941	28.193	1.00 26.85		N
ATOM	1847	CA			356	68.075	50.008	26.813	1.00 27.44		C
MOTA	1848	C			356	68.148	51.436	26.298	1.00 27.62		C
ATOM	1849	0			356	67.170	52.177	26.385	1.00 28.60		0
MOTA	1850	CB			356	67.099	49.198	25.945	1.00 28.37		C
ATOM	1851	SG			356	67.313	49.376	24.155	1.00 31.02		S
MOTA	1852	N			357	69.305	51.826	25.770	1.00 27.52		N
MOTA	1853	CA			357	69.455	53.160	25.196	1.00 28.11		С
MOTA	1854	С			357	68.975	52.992	23.756	1.00 28.62		C
MOTA	1855	0			357	69.628	52.323	22.948	1.00 28.65		0
MOTA	1856	CB			357	70.916	53.610	25.210	1.00 27.16		C
MOTA	1857	OG			357	71.045	54.894	24.615	1.00 28.40		0
MOTA	1858	N			358	67.831	53.594	23.451	1.00 29.11		N
MOTA	1859	CA			358	67.215	53.487	22.124	1.00 30.39		C
MOTA	1860	С			358	67.269	54.773	21.294	1.00 30.74		С
MOTA	1861	0			358	66.604	55.758	21.608	1.00 29.70		0
MOTA	1862	CB	ASP	Α	358	65.762	53.019	22.305	1.00 29.62		C
MOTA	1863	CG			358	64.978	52.960	21.007	1.00 30.36		С
MOTA	1864	OD1	ASP	Α	358	65.580	52.835	19.920	1.00 31.20	•	0
ATOM	1865	OD2	ASP			63.734	53.022	21.086	1.00 30.14		0
MOTA	1866	N			359	68.081	54.751	20.240	1.00 33.56		N
MOTA	1867	CA	GLY	A	359	68.193	55.899	19.357	1.00 35.42		С
ATOM	1868	С	GLY	Α	359	69.310	56.878	19.659	1.00 38.10		C
MOTA	1869	0	GLY	Α	359	69.854	56.901	20.761	1.00 39.07		0
MOTA	1870	N	GLY	Α	360	69.662	57.681	18.659	1.00 40.00		N
ATOM	1871	CA	GLY	А	360	70.706	58.673	18.831	1.00 41.21		С
ATOM	1872	C	GLY	Α	360	72.123	58.198	18.581	1.00 41.96		С
MOTA	1873	0	GLY	Α	360	73.055	58.987	18.695	1.00 44.15		0
ATOM	1874	N			361	72.305	56.923	18.256	1.00 42.76		N
MOTA	1875	CA			361	73.646	56.410	17.996	1.00 43.52		С
MOTA	1876	C			361	74.052	56.802	16.581	1.00 44.42		С
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MOTA	1877	0	ILE			73.470	56.322	15.609		44.27		0
ATOM	1878	CB	ILE	Α	361	73.714	54.862	18.107	1.00	43.69		C
ATOM	1879	CG1	ILE	A	361	73.392	54.412	19.538	1.00	43.46		C
ATOM	1880	CG2	ILE			75.095	54.366	17.685		42.46		С
MOTA	1881	CD1	ILE			74.429	54.792	20.565		42.32		C
MOTA	1882	N	VAL			75.049	57.675	16.469		45.42		N
MOTA	1883	CA	VAL	A	362	75.529	58.118	15.166	1.00	45.68		С
MOTA	1884	C	VAL	Α	362	76.851	57.440	14.820	1.00	45.91		C
MOTA	1885	0	VAL	Α	362	77.035	56.969	13.696	1.00	46.38		0
MOTA	1886	CB	VAL			75.723	59.643	15.135	1.00	46.35		С
ATOM	1887		VAL			76.105	60.091	13.727		48.19		C
ATOM	1888		VAL			74.444	60.333	15.572		46.73		C
ATOM	1889	N	TYR			77.761	57.379	15.792		44.38		N
MOTA	1890	CA	TYR			79.067	56.759	15.589		43.12		C
MOTA	1891	С	TYR	Α	363	79.278	55.547	16.491	1.00	41.17		С
MOTA	1892	0	TYR	Α	363	78.599	55.387	17.501	1.00	40.86		0
MOTA	1893	CB	TYR	Α	363	80.176	57.771	15.862	1.00	46.18		C
MOTA	1894	CG	TYR	Α	363	80.072	59.040	15.052	1.00	49.95		C
MOTA	1895	CD1	TYR			80.052	59.001	13.659		52.89		C
ATOM	1896	CD2	TYR			80.012	60.283	15.677		51.68		c
ATOM	1897	CE1	TYR			79.978	60.171	12.905		55.23	•	C
ATOM	1898	CE2	TYR			79.938	61.462	14.934		54.25		C
MOTA	1899	CZ	TYR	Α	363	79.924	61.397	13.549	1.00	55.42		С
MOTA	1900	OH	TYR	A	363	79:872	62.556	12.803	1.00	58.12		0
MOTA	1901	N	ASP	Α	364	80.231	54.695	16.134	1.00	39.35		N
ATOM	1902	CA	ASP	A	364	80.507	53.523	16.953	1.00	38.37		С
MOTA	1903	С	ASP			80.828	53.907	18.396		36.34		C
ATOM	1904		ASP			80.378	53.245	19.331		37.10		0
ATOM	1905	CB	ASP			81.681	52.712	16.386		40.35		C
ATOM	1906	CG	ASP			81.347	52.031	15.068		41.28		C
ATOM	1907		ASP			80.207	51.547	14.912	1.00	39.82	-	0
ATOM	1908	OD2	ASP	Α	364	82.236	51.964	14.197	1.00	42.22		0
MOTA	1909	N	TYR	Α	365	81.594	54.978	18.587	1.00	33.88		· N
MOTA	1910	CA	TYR	Α	365	81.959	55.375	19.945	1.00	33.29		С
ATOM	1911	С	TYR			80.754	55.781	20.792		31.98		C
MOTA	1912	ō	TYR			80.827	55.776	22.016		30.93		Ō
ATOM	1913		TYR									
		CB				83.031	56.477	19.926		32.04		C
ATOM	1914	CG	TYR			82.536	57.903	19.814		35.20		C
MOTA	1915	CD1	TYR			82.298	58.677	20.954		34.49		C
ATOM	1916	CD2	TYR	A	365	82.362	58.501	18.567	1.00	35.46		C
ATOM	1917	CE1	TYR	А	365	81.905	60.016	20.849	1.00	36.12		С
MOTA	1918	CE2	TYR	Α	365	81.971	59.837	18.452	1.00	37.53		C
MOTA	1919	CZ	TYR			81.744	60.586	19.594		37.51		С
ATOM	1920	ОН	TYR			81.351	61.901	19.461		40.00		0
ATOM	1921	N	HIS			79.641	56.119	20.143		31.70		N
ATOM												
	1922		HIS			78.434	56.467	20.882		32.08		C
MOTA	1923	C	HIS			77.938	55.198	21.591		30.99		C
ATOM	1924	0	HIS			77.289	55.278	22.635		30.53		0
MOTA	1925	CB	HIS			77.336	57.002	19.947	1.00	32.20		С
MOTA	1926	CG	HIS	Α	366	77.597	58.378	19.422	1.00	33.31		С
MOTA	1927	ND1	HIS	A	366	78.598	59.190	19.914	1.00	34.60		N
MOTA	1928		HIS			76.948	59.110	18.485		33.99		C
ATOM	1929		HIS			78.552	60.362	19.305		32.63		C
MOTA	1930		HIS				60.339					
						77.560		18.434		35.91		N
MOTA	1931	N	MET			78.244	54.031	21.017		30.17		И
MOTA	1932		MET			77.853	52.748	21.619		30.37		C
MOTA	1933	C	MET	A	367	78.588	52.573	22.953	1.00	29.75		C

MOTA	1934	Ö	MET	A	367	77.997	52.214	23.967	1.00	31.07	0
MOTA	1935	CB	MET	Α	367	78.232	51.567	20.711	1.00	30.58	С
MOTA	1936	CG	MET	Α	367	77.477	51.457	19.385	1.00	31.52	С
MOTA	1937	SD	MET	Α	367	78.053	50.007	18.447		35.95	S
MOTA	1938	CE	MET	A	367	77.121	50.189	16.917	1.00	34.32	C
MOTA	1939	N	THR	A	368	79.894	52.810	22.928	1.00	29.18	N
MOTA	1940	CA	THR			80.726	52.688	24.118	1.00	29.61	C
MOTA	1941	C	THR	A	368	80.241	53.682	25.165	1.00	28.28	С
MOTA	1942	0	THR	Α	368	80.163	53.354	26.343	1.00	29.90	0
MOTA	1943	CB	THR	Α	368	82.196	52.974	23.775	1.00	29.95	C
ATOM	1944	OG1	THR			82.548	52.222	22.606		31.91	0
MOTA	1945	CG2	THR			83.113	52.574	24.928		28.50	C
MOTA	1946	N	LEU			79.916	54.895	24.729		28.13	N
ATOM	1947	CA	LEU			79.418	55.925	25.639		29.19	C
MOTA	1948	C	LEU			78.117	55.493	26.321		28.58	C
MOTA	1949	0	LEU			77.978	55.619	27.535		28.56	0
ATOM `	1950	CB	LEU			79.165	57.245	24.890		29.00	C
MOTA	1951	CG	LEU			80.362	58.150	24.593		30.35	C
MOTA	1952	CD1				79.877	59.404	23.866		30.34	C
ATOM	1953		LEU			81.064	58.528	25.898		28.91	C
MOTA	1954	N	ALA			77.172	54.990	25.529		28.37	N
MOTA	1955	CA	ALA			75.880	54.560	26.052		28.93	C
ATOM	1956	C	ALA			76.052	53.464	27.103		27.87	C
MOTA	1957	.0	ALA			75.424	53.500	28.152		28.49	0
ATOM	1958	CB	ALA			74.987	54.064	24.911		26.15	C
ATOM	1959	N	LEU			76.905	52.491	26.813		27.99	N
MOTA	1960	CA	LEU			77.146	51.401	27.746		28.20	C
ATOM	1961	C	LEU			77.852	51.935	28.995		28.01	C
ATOM	1962	0.	LEU			77.475	51.599	30.111		27.43	0
MOTA	1963	CB	LEU			77.992	50.309	27.069		27.75	C
MOTA	1964	CG	LEU			77.347	49.632	25.844		29.75	C
ATOM	1965	CD1	LEU			78.370	48.736	25.140		31.88 29.40	C
ATOM ATOM	1966 1967	N	LEU ALA			76.140 78.863	48.815 52.783	26.272 28.803		27.59	N
ATOM	1968	CA	ALA			79.608	53.346	29.923		27.55	, C
ATOM	1969	C	ALA			78.710	54.146	30.845		28.89	C
MOTA	1970	0	ALA			78.913	54.158	32.063		28.91	0
MOTA	1971	СВ			372	80.746	54.226	29.423		25.48	C
MOTA	1972	N	MET			77.723	54.828	30.271		28.54	N
ATOM	1973	CA	MET			76.813	55.616	31.090		28.48	C
ATOM	1974	C			373	75.815	54.738	31.853		28.37	C
ATOM	1975	0	MET			75.048	55.238	32.665		28.46	0
ATOM	1976	CB.	MET			76.084	56.655	30.229		26.76	C
ATOM	1977	CG	MET			76.992	57.775	29.722		26.55	C
ATOM	1978	SD	MET			76.204	58.784	28.435		29.55	s
ATOM	1979	CE	MET			77.549	59.940	27.986		27.96	С
ATOM	1980	N			374	75.825	53.430	31.606		28.86	N
ATOM	1981	CA			374	74.917	52.563	32.344		27.32	С
ATOM	1982	С			374	73.906	51.744	31.563		28.78	С
ATOM	1983	0			374	73.257	50.862	32.133		29.86	0
ATOM	1984	N			375	73.746	52.023	30.274		27.82	N
ATOM	1985	CA			375	72.812	51.249	29.472	1.00	28.98	С
MOTA	1986	С	ALA	Α	375	73.363	49.829	29.355	1.00	29.41	С
MOTA	1987	0			375	74.552	49.641	29.099		30.88	0
MOTA	1988	CB	ALA	A	375	72.657	51.866	28.086	1.00	26.18	С
MOTA	1989	N	ASP	Α	376	72.500	48.837	29.545		29.,72	N
MOTA	1990	CA	ASP	A	376	72.900	47.435	29.457	1.00	30.17	C

MOTA	1991	С	ASP	Α	376	72.997	47.034	27.994	1.00	30.68		С
MOTA	1992	0	ASP	Α	376	73.896	46.293	27.597	1.00	30.02		0
ATOM	1993	CB	ASP	Α	376	71.882	46.568	30.187	1.00	30.75		С
ATOM	1994	CG			376	71.780	46.924	31.658		31.02		С
ATOM	1995		ASP			72.596	46.409	32.455		29.99		Ō
ATOM	1996		ASP			70.895	47.733	32.013		31.49		0
MOTA	1997	N			377	72.058	47.513	27.189		30.61		N
ATOM	1998	CA			377	72.106	47.236	25.767		30.87		C
MOTA	1999	C			377	71.603	48.425	24.954		30.14		С
MOTA	2000	0			377	71.047	49.388	25.498		29.61		0
MOTA	2001	CB	PHE	Α	377	71.374	45.922	25.396	1.00	29.78		С
ATOM	2002	CG			377	69.955	45.827	25.881	1.00	31.57		C
ATOM	2003	CD1	PHE	Α	377	69.673	45.401	27.178	1.00	31.78		C
ATOM	2004	CD2	,PHE	Α	377	68.894	46.099	25.020	1.00	31.27		C
MOTA	2005	CE1	PHE	Α	377	68.349	45.242	27.610	1.00	32.32		C
MOTA	2006		PHE			67.569	45.945	25.436		32.45		C
ATOM	2007	CZ			377	67.295	45.514	26.735		32.96		C
ATOM	2008	N			378	71.820	48.354	23.648		30.17		N
ATOM	2009	CA			378	71.473	49.436	22.742		30.04		C
MOTA	2010	C			378					30.86		C
						70.520	49.007	21.627				
ATOM	2011	0			378	70.693	47.939	21.038		31.49		0
	2012	CB			378	72.772	49.974	22.099		31.01		C
ATOM	2013	CG1			378	73.760	50.360	23.201		32.35		С
MOTA	2014		ILE			72.482	51.174	21.191	1.00	31.58		C
MOTA	2015	CD1	ILE			75.178	50.566	22.694	1.00	34.75		C
MOTA	2016	N	MET	Α	379	69.511	49.829	21.349	1.00	29.83		N
ATOM	2017	CA	MET	Α	379	68.581	49.531	20.265	1.00	30.54		C
MOTA	2018	С	MET	Α	379	68.913	50.461	19.095	1.00	30.14		С
ATOM	2019	0			379	69.010	51.669	19.268		29.93		0
ATOM	2020	СВ			379	67.122	49.749	20.694		30.89		C
ATOM	2021	CG			379	66.139	49.547	19.538		31.32		C
ATOM	2022	SD			379	64.386	49.460	19.961		31.78		s
MOTA	2023	CE			379	64.246	47.743	20.461		30.99		C
ATOM												
	2024	N			380	69.090	49.901	17.906		30.34		N
ATOM	2025	CA			380	69.416	50.720	16.746		31.69		C
MOTA	2026	·C			380	68.521	50.429	15.553		31.86		C
MOTA	2027	0			380	68.100	49.293	15.343		31.20		0
MOTA	2028	CB			380	70.879	50.514	16.331		31.86		С
MOTA	2029	CG			380	71.975	50.752	17.373		33.23	 	C
ATOM	2030		LEU			72.067	49.532	18.282	1.00	34.47		С
ATOM	2031	CD2	LEU	А	380	73.319	50.966	16.679	1.00	33.89		C
MOTA	2032	N	GLY	Α	381	68.241	51.469	14.775	1.00	32.46		N
MOTA	2033	CA	GLY	Α	381	67.414	51.321	13.589	1.00	33.27		C
MOTA	2034	C	GLY	Α	381	68.237	51.561	12.338	1.00	34.20		C
MOTA	2035	0			381	68.519	50.635	11.580		34.83		0
MOTA	2036	N			382	68.630	52.813	12.132		35.93		N
ATOM	2037	CA			382	69.431	53.220	10.978		37.19		C
ATOM	2038	C			382	70.643	52.297	10.765		36.78		C
ATOM	2039	0			382	70.879	51.801	9.660		35.86		0
ATOM	2040	CB			382	69.905	54.666	11.181		39.94		C
ATOM	2041	CG			382	70.739	55.238	10.039		45.52		C
MOTA	2042	CD			382	71.468	56.513	10.466		49.66		С
MOTA	2043	NE			382	72.418	56.259	11.552		53.52		N
MOTA	2044	CZ			382	73.540	55.552	11.423		54.96		C
MOTA	2045		ARG			73.871	55.023	10.249	1.00	54.91		N
MOTA	2046	NH2	ARG	A	382	74.327	55.359	12.478	1.00	54.92		N
MOTA	2047	N	TYR	A	383	71.405	52.080	11.834	1.00	35.43		N

MOTA	2048	CA	TYR	A	383		72:595	51.230	11.798	1.00 34.40	С
MOTA	2049	C	TYR	A	383		72.324	49.893	11.108	1.00 34.58	C
ATOM	2050	0	TYR	Α	383		73.082	49.480	10.229	1.00 35.55	0
ATOM	2051	CB	TYR	Α	383		73.091	50.975	13.230	1.00 32.13	С
ATOM	2052	CG	TYR	A	383		74.315	50.090	13.328	1.00 32.06	С
ATOM	2053.	CD1	TYR				75.603	50.628	13.275	1.00 31.61	С
ATOM	2054	CD2	TYR				74.185	48.711	13.476	1.00 31.52	С
MOTA	2055	CE1	TYR				76.728	49.811	13.370	1.00 32.15	C
ATOM	2056	CE2	TYR			•	75.293	47.889	13.569	1.00 30.67	c
ATOM	2057	CZ	TYR				76.564	48.440	13.516	1.00 33.10	Ċ
ATOM	2058	OH	TYR				77.662	47.610	13.604	1.00 30,90	. 0
ATOM	2059	N			384		71.242	49.227	11.505	1.00 32.76	N
ATOM	2060	CA	PHE				70.877	47.929	10.936	1.00 34.01	C
ATOM	2061	C	PHE				70.164	47.997	9.574	1.00 34.71	c
ATOM	2062	0	PHE				70.249	47.058	8.782	1.00 34.71	0
MOTA	2063	CB	PHE				70.004	47.150	11.930	1.00 33.23	C
ATOM	2063	CG	PHE				70.764				C
ATOM								46.603	13.115	1.00 33.56	
	2065		PHE				71.737	45.618	12.944	1.00 32.15	C
MOTA	2066		PHE			•	70.510	47.076	14.401	1.00 31.87	C
MOTA	2067		PHE				72.447	45.113	14.037	1.00 32.91	C
MOTA	2068		PHE				71.211	46.579	15.497	1.00 32.18	C
ATOM	2069	CZ	PHE				72.181	45.596	15.317	1.00 31.64	C
ATOM	2070	N	ALA				69.465	49.096	9.305	1.00 35.43	N
MOTA	2071	CA	ALA				68.750	49.250	8.036	1.00 36.93	С
MOTA	2072	C	ALA				69.702	49.171	6.842	1.00 37.68	С
MOTA	2073	0	ALA				69.335	48.678	5.776	1.00 37.47	0
MOTA	2074	CB	ALA				67.999	.50.585	8.014	1.00 35.75	С
MOTA	2075	N	ARG				70.926	49.658	7.038	1.00 38.60	N
MOTA	2076	CA	ARG				71.956	49.672	6.001	1.00 38.80	C
MOTA	2077	C	ARG	Α	386		72.388	48.285	5.532	1.00 39.38	С
MOTA	2078	0	ARG	Α	386		73.027	48.151	4.482	1.00 39.24	0
ATOM	2079	CB	ARG	Α	386		73.213	50:392	6.506	1.00 38.96	C
MOTA	2080	CG	ARG	A	386		73.057	51.842	6.915	1.00 41.08	С
MOTA	2081	CD	ARG	Α	386		74.373	52.314	7.530	1.00 43.49	C
MOTA	2082	NE	ARG	Α	386		74.784	51.422	8.616	1.00 45.03	N
MOTA	2083	CZ	ARG	Α	386		76.045	51.162	8.950	1.00 45.42	C
MOTA	2084	NHl	ARG	Α	386		77.049	51.724	8.284	1.00 44.14	N
MOTA	2085	NH2	ARG	Α	386		76.301	50.330	9.954	1.00 44.38	N
ATOM	2086	N	PHE	Α	387		72.057	47.256	6.302	1.00 40.14	N
ATOM	2087	CA	PHE	Α	387		72.483	45.911	5.950	1.00 41.48	С
ATOM	2088	C	PHE	Α	387		71.620	45.137	4.954	1.00 43.09	С
ATOM	2089	0			387		70.412	45.350	4.827	1.00 43.30	. 0
MOTA	2090	СВ	PHE	Α	38.7		72.658	45.066	7.218	1.00 41.15	С
ATOM	2091	CG			387		73.559	45.690	8.255	1.00 41.44	С
ATOM	2092		PHE				74.665	46.450	7.878	1.00 40.93	C
ATOM	2093		PHE				73.312	45.496	9.614	1.00 40.05	C
MOTA	2094		PHE				75.512	47.007	8.837	1.00 40.83	C
ATOM	2095		PHE				74.154	46.048	10.583	1.00 39.34 .	C
ATOM	2096	CZ			387		75.254	46.804	10.196	1.00 39.79	C
ATOM	2097	N			388		72.284	44.222	4.261	1.00 44.03	N
ATOM	2098	CA	GLU				71.673	43.348	3.274	1.00 45.03	C
ATOM	2099	C	GLU				70.445	42.655	3.850	1.00 44.35	C
ATOM	2100	0	GLU				69.431	42.507	3.171	1.00 43.66	0
ATOM	2100	CB			388		72.700	42.297	2.846	1.00 46.61	c
ATOM	2101	CG			388		72.700	42.257	1.853	1.00 46.61	C
ATOM	2102	CD			388			41.252	0.516	1.00 50.47	C
ATOM			GLU				71.843				
AIOM	2104	OFI	GTO	М	200	•	72.569	42.769	0.063	1.00 54.19	0

ATOM	2105	OE2	GLU	Α	388	70.842	41.407	-0.089	1.00	54.15		0
MOTA	2106	N	GLU	Α	389 .	70.535	42.250	5.114	1.00	43.43		N
MOTA	2107	CA	GLU	Α	389	69.442	41.540	5.762	1.00	42.71		С
MOTA	2108	С	GLU	Α	389.	68.218	42.345	6.187	1.00	42.10		С
ATOM	2109	0			389	67.249	41.765	6.663	1.00	41.97		0
ATOM	2110	CB			389	69.973	40.738	6.955	1.00			C
ATOM	2111	CG			389	71.002	39.695	6.563	1.00			Ċ
ATOM	2112	CD			389	72.429	40.180	6.750	1.00			Ĉ
ATOM	2113	OE1				72.688	41.387	6.567	1.00			Ö
ATOM	2114	OE2				73.297	39.344	7.074	1.00			0
							43.666	6.041	1.00			N
ATOM	2115	N			390	68.245						
ATOM	2116	CA			390	67.065	44.446	6.399	1.00			C
ATOM	2117	C			390	66.047	44.174	5.280	1.00			C
ATOM	2118	0			390	66.422	44.044	4.112	1.00			0
MOTA	2119	CB			390	67.387	45.938	6.492	1.00			С
MOTA	2120	OG			390	67.730	46.469	5.230	1.00			0
ATOM	2121	N			391	64.750	44.096	5.625	1.00			N
MOTA	2122	CA	PRO	А	391	63.649	43.825	4.690	1.00	50.18		C
MOTA	2123	C	PRO	Α	391	63.348	44.842	3.587	1.00	51.58		С
ATOM	2124	0	PRO	A	391	62.530	44.575	2.707	1.00	53.10		0
MOTA	2125	CB	PRO	A	391	62.459	43.632	5.626	1.00	49.90	* .	C
ATOM	2126	CG	PRO	Α	391	62.741	44.643	6.698	1.00	48.60		С
MOTA	2127	CD	PRO	Α	391	64.223	44.439	6.962	1.00	47.30		С
ATOM	2128	N	THR	Α	392	63.996	45.998	3.623	1.00			N
ATOM	2129	CA			392	63.737	47.020	2.620	1.00			С
ATOM	2130	C			392	64.409	46.724	1.287	1.00			C
ATOM	2131	ō			392	65.163	45.759	1.158	1.00			o
ATOM	2132	СВ			392	64.186	48.403	3.114	1.00			C
ATOM	2132	OG1			392	65.610	48.421	3.263	1.00			0
ATOM									1.00			· C
	21,34		THR			63.528	48.719	4.455	1.00			N
ATOM	2135	N Cr			393	64.132	47.565	0.295				C
ATOM	2136	CA	ARG			64.699	47.376.		1.00			
ATOM	2137	C			393	66.023	48.088	-1.244	1.00			C
ATOM	2138	0	ARG			66.223	49.219	-0.800	1.00			0
MOTA	2139	CB			393	63.701	47.818	-2.112	1.00			C
MOTA	2140	CG			393	62.463	46.928	-2.205	1.00		•	С
MOTA	2141	CD			393	61.561	47.293	-3.386	1.00			С
MOTA	2142	NE			393	61.125	48.684	-3.338	1.00			N
MOTA	2143	CZ	ARG	Α	393	61.584	49.639	-4.139	1.00	67.03		C
MOTA	2144		ARG			62.495	49.355	-5.063	1.00			- N
MOTA	2145	NH2	ARG	Α	393	61.144	50.883	-4.006	1.00	67.53		N
MOTA	2146	N	LYS	Α	394	66.927	47.394	-1.925	1.00	59.11		N
MOTA	2147	CA	LYS	Α	394	68.241	47.922	-2.248	1.00	59.88		C
ATOM	2148	C	LYS	Α	394	68.034	48.693	-3.542	1.00	60.73		С
MOTA	2149	Ö	LYS	Α	394	67.680	48.106	-4.562	1.00	61.24		0
ATOM	2150	CB			394	69.218	46.768	-2.479	1.00	59.07		C
MOTA	2151	CG			394	70.646	47.055	-2.060	1.00	58.59		С
MOTA	2152	CD			394	71.590	45.945	-2.504	1.00			С
ATOM	2153	CE			394	71.164	44.582	-1.990	1.00			С
ATOM	2154	NZ			394	72.088	43.519	-2.476	1.00			N
	2155	N			395	68.234	50.005	-3.503	1.00			, N.
ATOM	2156	CA			395	68.048	50.827	-4.692	1.00			C
ATOM	2157	C			395	69.326	51.564	-5.069	1.00			C
ATOM												0
	2158	O			395	69.995	52.143	-4.215		65.50		C
ATOM	2159	CB CC1			395	66.917	51.859	-4.483	1.00			
ATOM	2160		VAL			65.642	51.147	-4.064	1.00			C
MOTA	2161	CG2	VAL	A	395	67.323	52.884	-3.438	1.00	63.76		С

ATOM	2162	N	THR	Α	396	69.666	51.537	-6.354	1.00 66.43	3	N.
ATOM	2163	CA	THR	Α	396	70.869	52.209	-6.829	1.00 67.58	3	С
MOTA	2164	C	THR	Α	396	70.552	53.613	-7.319	1.00 68.48	3	C
MOTA	2165	0	THR	Α	396	69.742	53.799	-8.227	1.00 68.56	5	0
ATOM	2166	CB `	THR	Α	396	71.535	51.427	-7.971	1.00 67.68	3	С
ATOM	2167	OG1	THR	A	396	71.919	50.130	-7.500	1.00 68.09	9	0
ATOM	2168	CG2	THR	Α	396,	72.773	52.162	-8.464	1.00 68.17	7	C
ATOM	2169	N	ILE			71.198	54.599	-6.707	1.00 69.55	5	N
ATOM	2170	CA	ILE			70.999	55.996	-7.066	1.00 70.46	5	C
ATOM	2171	С	ILE			72.322	56.609	-7.518	1.00 71.03		С
ATOM	2172	0	ILE			73.224	56.826	-6.708	1.00 71.53	3	0
ATOM	2173	СВ	ILE			70.453	56.791	-5.867	1.00 70.76		C
ATOM	2174	CG1				69.148	56.154	-5.384	1.00 71.18		С
ATOM	2175		ILE			70.231	58.246	-6.259	1.00 70.80		C
ATOM	2176		ILE			68.542	56.832	-4.175	1.00 71.99		C
ATOM	2177	N	ASN			72.425	56.879	-8.817	1.00 71.4		N
ATOM	2178	CA	ASN			73.624	57.464	-9.417	1.00 71.04		C
		C	ASN			74.940	56.865	-8.914	1.00 69.90		C
ATOM	2179						57.574	-8.389	1.00 69.7		0
ATOM	2180	0	ASN			75.802		-9.218	1.00 03.7		C
ATOM	2181	CB	ASN			73.630	58.989				C
ATOM	2182	CG	ASN			73.544	59.397	-7.755	1.00 74.8		
ATOM	2183		ASN			74.421	59.071	-6.949	1.00 76.2		0
ATOM	2184		ASN			72.483	60.119	-7.406	1.00 75.3		N
ATOM	2185	N	GLY			75.088	55.554	-9.082	1.00 68.28		N
ATOM	2186	CA	GLY			76.307	54.885	-8.659	1.00 66.7		C
ATOM	2187	C	GLY			76.392	54.549	-7.181	1.00 65.5		C
ATOM	2188	0	GLY			77.351	53.912	-6.739	1.00 65.5		0
MOTA	2189	N	SER	Α	400	75.398	54.976	-6.410	1.00 63.83		N
MOTA	2190	CA	SER	А	400	75.391	54.697	-4.980	1.00 61.7		С
MOTA	2191	C	SER	Α	400	74.256	53.761	-4.602	1.00 59.9	3	С
ATOM	2192	0	SER	Α	400	73.086	54.095	-4.768	1.00 60.3	5	0
ATOM	2193	CB	SER	Α	4Ò0	75.267	55.997	-4.185	1.00 61.2	9	С
MOTA	2194	OG	SER	Α	400	76.440	56.778	-4.317	1.00 62.1	5	0
MOTA	2195	N	VAL	A	401	74.606	52.583	-4.101	1.00 58.0	9	N
ATOM	2196`	CA	VAL	Α	401	73.602	51.617	-3.685	1.00 56.6	2	C
ATOM.	2197	C	VAL	A	401	73.099	52.029	-2.303	1.00 56.9	6	С
ATOM	2198	0	VAL	Α	401	73.886	52.176	-1.361	1.00 57.5	5	0
MOTA	2199	CB	VAL	A	401·	74.190	50.198	-3.621	1.00 56.1	9	С
ATOM	2200	CG1	VAL	Α	401	73.129	49.214	-3.161	1.00 54.6	3	C
ATOM	2201	CG2	VAL	A	401	74.729	49.805	-4.992	1.00 55.0	2	C
ATOM	2202	N			402	71.789	52.226	-2.190	1.00 55.3	6	N
ATOM	2203	CA			402	71.181	52.648	-0.935	1.00 53.8	4	C
ATOM	2204	C.			402	70.113	51.661	-0.482	1.00 52.6		С
ATOM	2205		MET			69.789	50.707	-1.188	1.00 51.8		0
ATOM	2206	CB			402	70.521	54.022	-1.109	1.00 55.2		С
ATOM	2207	CG			402	71.356	55.062	-1.837	1.00 55.3		C
ATOM	2208	SD			402	72.760	55.653	-0.884	1.00 59.3		S
ATOM	2209	CE			402	71.959	56.904	0.134	1.00 56.8		C
ATOM	2210	N			403	69.579	51.900	0.713	1.00 50.1		· N
ATOM	2211	CA			403	68.506	51.082	1.258	1.00 48.1		C
ATOM	2212	C			403	67.452	52.043	1.791	1.00 47.2		C
MOTA	2212	0			403	67.776	53.124	2.285	1.00 47.2		0
							50.168	2.382	1.00 48.1		C
ATOM	2214	CB			403	69.007		1.921	1.00 48.4		C
ATOM	2215	CG			403	69.976	49.093		1.00 48.7		C
ATOM	2216	CD			403	69.677	47.739	2.552			C
ATOM	2217	CE			403	68.415	47.121	1.972	1.00 48.7		
ATOM	2218	NZ	LYS	A	403	68.133	45.771	2.538	1.00 47.6	D .	N

MOTA	2219	N	GLU	А	404	66.189	51.660	1.674	1.00	46.83		N
ATOM	2220	CA	GLU	A	404	65.115	52.514	2.147	1.00	46.62		С
ATOM	2221	С	GLU	Α	404	65.046	52.448	3.661	1.00	45.53		C
MOTA	2222	0	GLU	Α	404	65.329	51.412	4.269	1.00	43.78		0
ATOM	2223	CB	GLU			63.776	52.064	1.582		49.02		С
ATOM	2224	CG	GLU			63.846	51.421	0.222	•	53.76		C
ATOM	2225	CD	GLU			62.473 .		-0.291		55.98		C
ATOM	2226		GLU			61.767	51.971	-0.772		56.94		0
MOTA	2227	OE2	GLU			62.100	49.863	-0.193		57.61		0
ATOM	2228	N	TYR			64.661	53.560	4.268		44.22		N
ATOM	2229	CA	TYR			64.543	53.615	5.708		43.49		С
MOTA	2230	C	TYR			63.488	54.634	6.071		42.96		C
ATOM	2231	0	TYR			63.612	55.811	5.744		43.26		0
ATOM	2232	СВ	TYR			65.883	53.992	6.341		43.62		C
ATOM	2233	CG	TYR			65.853	54.018	7.851		43.93		C
ATOM	2234		TYR			65.416	52.913	8.579		42.98		C
ATOM	2235	CD2	TYR			66.258	55.150	8.554		44.65		C
ATOM	2236	CE1	TYR			65.380	52.938	9.972		44.02	•	C
ATOM	2237	CE2	TYR			66.227	55.184	9.946		44.86		C
ATOM	2238	CZ	TYR			65.786	54.077	10.646		43.66	•.	C
ATOM	2239	OH			405	65.736	54.126	12.018		43.77		0
ATOM	2240	N			406	62.438	54.171	6.738		41.92		N C
ATOM	2241	CA			406	61.361	55.052	7.149		40.62		C
ATOM	2242	C			406	60.985 61.088	54.760	8.594		40.02		0
ATOM	2243	O			406		53.622	9.056		38.27		C
ATOM	2244	CB	TRP			60.147	54.878	6.214		35.96		C
ATOM ATOM	2245 2246	CG CD1	TRP		406	59.520 58.543	53.510 53.065	6.228 7.074		35.90		C
	2247	CD1	TRP			59.845	52.405	5.373		35.52		C
ATOM	2247	NE1	TRP			58.239	51.752	6.800		36.00		N
ATOM ATOM	2249		TRP			59.024	51.732	5.762		36.30		C
ATOM	2250	CE3	TRP			60.750	52.225	4.315		36.42		C
ATOM	2251	CZ2			406	59.079	50.068	5.130		35.10		C
ATOM	2252	CZ3	TRP			60.806	50.979	3.683		35.93		C
ATOM	2253	CH2				59.972	49.918	4.096		35.80		Ċ
AŢOM	2254	N			407	60.568	55.800	9.307		41.39		N
ATOM	2255	CA			407	60.178	55.640	10.693		42.59		C
ATOM	2256	C			407	58.772	55.085	10.825		43.19		C
ATOM	2257	0			407	57.991	55.101	9.874		43.52		0
ATOM	2258	N			408-	58.452	54.589			43.79		N
ATOM	2259	CA			408	57.138	54.029	12.287		43.77		C
ATOM	2260	С			408	56.100	55.139	12.370		45.22		С
ATOM	2261	0	GLU	Α	408	54.899	54.891	12.292	1.00	45.34		0
ATOM	2262	CB	GLU	Α	408	57.181	53.252	13.599	1.00	42.61		C
MOTA	2263	CG	GLU	А	408	58.025	51.997	13.524	1.00	41.23		C
ATOM	2264	CD	GLU	A	408	57.372	50.920	12.674	1.00	39.91	•	С
MOTA	2265	OE1	GLU	A	408	56.280	50.456	13.056	1.00	39.37		0
ATOM	2266	OE2	GLU	Α	408	57.944	50.540	11.632	1.00	39.32		0
MOTA	2267	N	GLY	Α	409	56.576	56.368	12.529	1.00	46.42		N
ATOM	2268	CA	GLY	А	409	55.676	57.500	12.619	1.00	48.58		С
MOTA	2269	C	GLY	A	409	55.339	58.095	11.265	1.00	49.72		С
ATOM	2270	0	GLY	A	409	54.491	58.977	. 11.174	1.00	49.49		0
ATOM	2271	N	SER	A	410	56.001	57.628	10.210		51.57		N
MOTA	2272	CA	SER	A	410	55.725	58.151	8.876		53.58		С
MOTA	2273	C			410	54.411	57.566	8.385		55.64		С
MOTA	2274	0			410	54.006	56.486	8.816		54.76		0
MOTA	2275	CB	SER	A	410	56.849	57.791	7.899	1.00	53.27		C

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MOTA	2276	OG	SER	Α	410	56.837	56.411	7.578	1.00 54.06	0
MOTA	2277	N	SER	A	411	53.740	58.285	7.490	1.00 58.45	N
ATOM	2278	CA	SER	A	411	52.472	57.816	6.951	1.00 61.28	C
ATOM	2279	C	SER	A	411	52.689	56.508	6.199	1.00 62.71	C
ATOM	2280	0	SER	Α	411	51.794	55.662	6.123	1.00 62.97	0
ATOM	2281	CB	SER			51.875	58.873	6.020	1.00 62.05	. C
ATOM	2282	OG	SER			52.807	59.264	5.028	1.00 63.19	0
ATOM	2283	N	ARG			53.892	56.343	5.658	1.00 64.06	N
MOTA	2284	CA	ARG			54.241	55.141	4.910	1.00 65.82	С
		C	ARG			54.229	53.882	5.776	1.00 67.23	Ċ
ATOM	2285					54.157	52.768	5.259	1.00 66.85	Ō
ATOM	2286	0	ARG				55.306	4.273	1.00 64.77	C
ATOM	2287	CB	ARG			55.626	54.068	3.544	1.00 63.53	c
ATOM	2288	CG	ARG			56.114			1.00 62.50	C
MOTA	2289	CD.	ARG			57.441	54.298	2.845		
ATOM	2290	NE	ARG			57.882	53.089	2.155	1.00 61.94	N G
MOTA	2291	CZ	ARG			58.990	52.996	1.429	1.00 62.83	C
MOTA	2292		ARG			59.791	54.047	1.286	1.00 62.91	N
MOTA	2293	NH2	ARG			59.298	51.846	0.842	1.00 62.91	- N
MOTA	2294	N	ALA.	Α	413	54.285	54.065	7.093	1.00 69.94	N
ATOM	2295	CA	ALA	Α	413	54.315	52.940	8.022	1.00 72.61	С
ATOM	2296	C	ALA	А	413	52.973	52.554	8.631	1.00 74.53	C
MOTA	2297	0	ALA	Α	413	52.439	51.485	8.337	1.00 74.51	0
MOTA	2298	CB	ALA	Α	413	55.323	53.221	9.138	1.00 71.60	C
MOTA	2299	N	ARG	Α	414	52.434	53.419	9.487	1.00 77.76	N
ATOM	2300	CA	ARG		,	51.167	53.137	10.155	1.00 80.61	C
ATOM	2301	C			414	49.963	53.024	9.213	1.00 81.50	C
ATOM	2302	0	ARG			48.815	53.073	9.661	1.00 81.79	0
ATOM	2303	CB	ARG			50.893	54.184	11.247	1.00 81.68	C
ATOM	2304	CG	ARG			50.556	55.589	10.755	1.00 83.90	C
ATOM	2305	CD	ARG			50.207	56.490	11.941	1.00 85.67	С
ATOM	2306	NE			414	49.470	57.693	11.558	1.00 87.41	N
ATOM	2307	CZ			414	48.918	58.537	12.426	1.00 88.02	C
ATOM	2308		ARG			49.021	58.312	13.731	1.00 87.96	N
ATOM	2309		ARG			48.253	59.602	11.994	1.00 88.30	N
		N			415	50.226	52.867	7.916	1.00 82.42	N
MOTA	2310				415	49.152	52.714	6.932	1.00 82.74	C
MOTA	2311	CA						6.722	1.00 83.26	C
ATOM	2312	C			415	48.897	51.218	5.583	1.00 82.62	0
MOTA	2313	0			415	48.846	50.745			
MOTA	2314	·CB	ASN	•		49.535	53.345	5.581	1.00 83.10	C
MOTA	2315	CG			415	48.309		4.757	1.00 83.44	
MOTA	2316		ASN			48.403	53.990	3.538	1.00 81.84	0
MOTA	2317	ND2			415	47.148	53.894		1.00 83.48	N
MOTA	2318	N			416	48.751	50.476	7.819	1.00 83.43	N
MOTA	2319	CA			416	48.504	49.039	7.734	1.00 83.29	C
MOTA	2320	C			416	47.153	48.658	8.340	1.00 83.50	С
MOTA	2321	0	TRP	Α	416	46.650	49.328	9.246	1.00 83.70	0
MOTA	2322	CB	TRP	Α	416	49.622	48.251	8.435	1.00 83.05	C
ATOM	2323	CG	TRP	Α	416	49.577	48.306	9.936	1.00 83.22	C
MOTA	2324	CD1	TRP	Α	416	50.081	49.288	10.742	1.00 83.70	C
MOTA	2325	CD2	TRP	A	416	48.957	47.350	10.807	1.00 83.09	C
ATOM	2326		TRP			49.812	49.003	12.062	1.00 83.83	· N
MOTA	2327		TRP			49.122	47.820	12.130	1.00 83.53	C
MOTA	2328		TRP			48.274	46.143	10.597	1.00 82.77	C
ATOM	2329		TRP			48.629	47.123	13.240	1.00 83.40	С
ATOM	2330		TRP			47.784	45.452	11.699	1.00 82.88	С
ATOM	2331				416	47.965	45.945	13.005	1.00 83.24	C
ATOM	2331	N			431	55.027	62.893	11.346	1.00 77.68	N
AION	256	7.4	GILO	~	171	55.027	02.000	510		•,

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ATOM	2333	CA	GLU	Α	431	55.426	62.297	12.617	1.00 77.79			С
MOTA	2334	С	GLU	Α	431	56.719	61.495	12.439	1.00 76.90			С
MOTA	2335	0	GLU	Α	431	57.500	61.317	13.379	1.00 77.08			0
ATOM	2336	CB	GLU			54.302	61.396	13.140	1.00 79.27			С
ATOM	2337	CG	GLU			52.947	62.100	13.227	1.00 81.73			С
ATOM	2338	CD	GLU			51.852	61.222	13.817	1.00 83.20			С
			GLU			51.961	60.841	15.004	1.00 83.92			0
ATOM	2339							13.093	1.00 83.75			0
MOTA	2340				431	50.881	60.914			•		N
MOTA	2341	N	GLY			56.936.		11.218	1.00 75.40			
ATOM	2342	CA	GLY			58.133	60.258	10.909	1.00 73.03			C
MOTA	2343	С	GLY	A	432	58.611	60.653	9.525	1.00 71.34			С
ATOM	2344	0	GLY	Α	432	57.915	61.386	8.818	1.00 71.32			0
ATOM	2345	N	VAL	А	433	59.789	60.179	9.130	1.00 69.14			N
ATOM	2346	CA	VAL	А	433	60.319	60.512	7.813	1.00 66.51			C
ATOM	2347	С	VAL	A	433	60.700	59.280	6.994	1.00 64.72			C
ATOM	2348	0	VAL			60.990	58.216	7.543	1.00 64.04			0
ATOM	2349	СВ	VAL			61.551	61.445	7.924	1.00 66.56			С
ATOM	2350		VAL			61.165	62.728	8.642	1.00 66.22			C
	2351		VAL			62.676	60.743	8.658	1.00 66.90			C
ATOM							59.446	5.675	1.00 62.15			N
ATOM	2352	N .	ASP			60.683						C
ATOM	2353	CA	ASP			61.019	58.387	4.732	1.00 59.84			C
MOTA	2354	C	ASP			62.320	58.807	4.046	1.00 58.55			
MOTA	2355	0	ASP			62.383	59.876	3.441	1.00 58.58			0
MOTA	2356	CB	ASP			59.894	58.247	3.699	1.00 59.57			C
MOTA	2357	CG	ASP	A	434	60.072	57.047	2.795	1.00 59.49			С
MOTA	2358	OD1	ASP	A	434	59.322	56.927	1.804	1.00 59.07			0
MOTA	2359	OD2	ASP	Α	434	60.959	56.217	<b>3.079</b>	1.00 60.22			0
MOTA	2360	N	SER	Α	435	63.355	57.976	4.136	1.00 56.49			N
ATOM	2361	CA	SER			64.641	58.320	3.537	1.00 54.56			С
ATOM	2362	C			435	65.459	57.138	3.031	1.00 52.57			C
ATOM	2363	0			435	64.954	56.028	2.890	1.00 51.40			0
ATOM	2364	CB			435	65.480	59.107	4.546	1.00 55.14			C
	2365	OG			435	65.660	58.357	5.736	1.00 56.74			0
ATOM					436	66.735	57.401	2.764	1.00 51.28			N
ATOM	2366	N							1.00 50.73			C
ATOM	2367	CA			436	67.664	56.391	2.269				C
MOTA	2368	С			436	68.936	56.359	3.114	1.00 50.04			
MOTA	2369	0			436	69.356	57.382	3.657	1.00 50.12			0
MOTA	2370	CB			436	68.057	56.704	0.824	1.00 52.87			C
MOTA		, CG	TYR	Α	436	66.940	56.591	-0.185	1.00 53.47			C
MOTA	2372	CD1	TYR	Α	436	66.475	55.344	-0.603	1.00 53.78		•	C
MOTA	2373	CD2	TYR	Α	436	66.356	57.733	-0.733	1.00 54.90			С
ATOM	2374	CE1	TYR	Α	436	65.457	55.237	-1.545	1.00 54.59			С
ATOM	2375	CE2	TYR	Α	436	65.333	57.637	-1.679	1.00 55.49			С
ATOM	2376	CZ	TYR	Α	436	64.891	56.386	-2.077	1.00 55.11			C
MOTA	2377	ОН			436	63.876	56.285	-2.999	1.00 56.28			0
ATOM	2378	N			437	69.541	55.180	3.227	1.00 47.66			N
ATOM	2379	CA			437	70.785	55.022	3.969	1.00 46.24			С
ATOM	2380	C			437	71.743	54.236	3.089	1.00 46.02			С
ATOM	2381	0			437	71.343	53.283	2.421	1.00 45.29			0
						70.592	54.260	5.314	1.00 46.00			C
MOTA	2382	CB			437			6.227	1.00 45.51			C
ATOM	2383		VAL			69.654	55.037					C
ATOM	2384		VAL			70.071	52.853	5.058	1.00 44.32			
ATOM	2385	N			438	73.026	54.628	3.073	1.00 46.55			N
MOTA	2386	CA			438	74.024	53.935	2.252	1.00 45.89			C
MOTA	2387	С			438	74.178	52.463	2.600	1.00 45.71			C
MOTA	2388	0	PRO	A	438	74.268	52.095	. 3.773	1.00 45.41			0
MOTA	2389	CB	PRO	A	438	75.301	54.738	2.506	1.00 46.50			C

ATOM	2390	CG	PRO	А	438	75.099	55.254	3.901	1.00 47.81	C
ATOM	2391	CD	PRO	А	438	73.652	55.688	3.881	1.00 46.25	С
ATOM	2392	N	TYR	Α	439	74.191	51.629	1.564	1.00 44.94	N
ATOM	2393	CA	TYR	Α	439	74.340	50.187	1.712	1.00 44.07	С
ATOM	2394	C	TYR			75.686	49.898	2.371	1.00 44.51	С
MOTA	2395	Ō	TYR			76.711	50.459	1.985	1.00 44.53	0
ATOM	2396	CB	TYR			74.273	49.521	0.334	1.00 42.82	C
ATOM	2397	CG	TYR			74.442	48.019	0.340	1.00 41.12	C
	2398	CD1	TYR			73.561	47.201	1.041	1.00 41.12	C
ATOM							47.412	-0.388	1.00 42.23	C
ATOM	2399	CD2	TYR			75.464	45.811		1.00 42.23	C
ATOM	2400	CE1	TYR			73.690		1.014		
MOTA	2401	CE2	TYR			75.603	46.025		1.00 42.30	C
MOTA	2402	CZ	TYR			74.712	45.232	0.281	1.00 42.80	C
ATOM	2403	OH	TYR			74.834	43.861	0.242	1.00 44.53	0
ATOM	2404	N	ALA			75.684	49.014	3.361	1.00 44.65	N
ATOM	2405	CA	ALA			76.914	48.689	4.067	1.00 44.96	C
ATOM	2406	С	ALA	Α	440	77.335	47.239	3.880	1.00 44.76	С
MOTA	2407	0	ALA	Α	440	78.424	46.847	4.294	1.00 45.32	0
ATOM	2408	CB	ALA	Α	440	76.751	49.001	5.549	1.00 44.41	C
ATOM	2409	N	GLY	Α	441	76.479	46.447	3.248	1.00 44.13	N
ATOM	2410	CA	GLY	Α	441	76.803	45.049	3.041	1.00 43.90	C
ATOM	2411	C	GLY	Α	441	76.135	44.176	4.087	1.00 43.49	C
ATOM	2412	0	GLY	Α	441	75.115	44.559	4.660	1.00 43.21	0
ATOM	2413	N	LYS	Α	442	76.713	43.005	4.341	1.00 44.00	N
ATOM	2414	CA	LYS			76.171	42.064	5.318	1.00 44.24	C
ATOM	2415	С	LYS			76.360	42.533	6.757	1.00 43.92	C
ATOM	2416	0	LYS	Α	442	77.363	43.171	7.091	1.00 44.02	0
ATOM	2417	CB	LYS			76.834	40.697	5.142	1.00 46.18	C
MOTA	2418	CG	LYS			76.608	40.085	3.766	1.00 50.07	C
ATOM	2419	CD	LYS			75.542	38.992	3.794	1.00 51.33	C
ATOM	2420	CE	LYS			76.086	37.716	4.431	1.00 54.42	C
ATOM	2421	NZ	LYS			75.115	36.573	4.373	1.00 55.91	N
ATOM	2422	N	LEU			75.393	42.200	7.605	1.00 42.94	N
ATOM	2423	CA	LEU			75.421	42.568	9.018	1.00 41.75	C
ATOM	2424	C	LEU			76.697	42.133	9.746	1.00 42.03	C
ATOM	2425	0	LEU			77.295	42.912	10.485	1.00 40.47	0
ATOM	2426	СВ	LEU			74.201	41.968	9.726	1.00 40.09	. C
ATOM	2427	CG	LEU			74.055	42.185	11.238	1.00 39.89	c
ATOM	2428		LEU			72.596	42.020	11.640	1.00 38.06	C
ATOM	2429				443	74.937	41.200	11.997	1.00 38.79	C
	2429				444	77.108		9.522	1.00 30.79	N
ATOM		N					40.315		1.00 42.70	C
ATOM	2431	CA			444					C
MOTA	2432	C			444		41.134	10.229	1.00 45.18	
MOTA	2433	0			444		41.445	11.314	1.00 44.50	0
ATOM	2434	CB			444		38.945	9.571	1.00 46.48	C
MOTA	2435	CG			444	79.616	38.150	10.374	1.00 50.45	C
MOTA	2436	CD			444	79.867	36.779	9.768	1.00 53.23	C
MOTA	2437	CE			444	80.731	35.935	10.688	1.00 54.88	C
MOTA	2438	NZ			444	82.030	36.605	10.975	1.00 55.49	N
MOTA	2439	N			445	80.134	41.466	9.068	1.00 45.06	N
MOTA	2440	CA			445	81.388	42.212	9.017	1.00 45.21	C
MOTA	2441	C			445	81.284	43.592	9.636	1.00 43.85	C
ATOM	2442	0			445		44.105	10.192	1.00 43.92	0
MOTA	2443	CB			445	81.880	42.349	7.573	1.00 48.38	C
ATOM	2444	CG	ASP	А	445		41.005	6.902	1.00 51.51	С
ATOM	2445	OD1	ASP	Α	445	82.776	40.133	7.507	1.00 52.73	0
MOTA	2446	OD2	ASP	A	445	81.620	40.825	5.766	1.00 53.93	0

ATOM	2447	N .	ASN	A	446		80.110	44.195	9.533		41.34		N
MOTA	2448	CA	ASN	А	446		79.900	45.522	10.086		40.70		С
ATOM	2449	C	ASN	Α	446		79.815	45.501	11.605	1.00	39.56		С
MOTA	2450	0	ASN	Α	446		80.439	46.318	12.273	1.00	40.02		0
MOTA	2451	CB	ASN	Α	446		78.637	46.126	9.491	1.00	40.72		C
ATOM	2452	CG	ASN				78.823	46.520	8.046	1.00	41.93		C
ATOM	2453		ASN				79.347	47.601	7.748	•	42.76		0
ATOM	2454		ASN				78.416	45.640	7.134		39.05		N
			VAL				79.039	44.571	12.146		38.14		N
ATOM	2455	N					78.901	44.450	13.590		38.14		C
MOTA	2456	CA	VAL								38.90		C
MOTA	2457	C	VAL				80.251	44.071	14.215				
ATOM	2458	0	VAL				80.594	44.534	15.295		38.04		0
ATOM	2459	CB	VAL				77.837	43.386	13.952		37.40		C
ATOM	2460		VAL				77.891	43.065	15.437		37.24		С
ATOM	2461	CG2	VAL	Α	447		76.454	43.899	13.579		36.23		C
ATOM	2462	N	GLU	Α	448		81.018	43.235	13.524	1.00	39.10		N
ATOM	2463	CA	GLU	Α	448	•	82.313	42.826	14.039	1.00	39.82		C
ATOM	2464	C	GLU	Α	448		83.247	44.036	14.100	1.00	37.84		C
MOTA	2465	0	GLU	A	448		83.963	44.222	15.078	1.00	36.51		0
ATOM	2466	CB	GLU	Α	448		82.917	41.728	13.153	1.00	42.41		С
ATOM	2467	CG			448		84.226	41.149	13.677	1.00	48.39		C
ATOM	2468	CD	GLU		•		84.802	40.073	12.760		53.42		С
ATOM	2469	OE1					85.409	40.422	11.718		53.76		ō
ATOM	2470	OE2	GLU				84.634		13.078		56.37		ō
								44.854	13.078		36.52		N
ATOM	2471	N	ALA				83.235						C
ATOM	2472	CA			449		84.081	46.045	13.006		36.71		
ATOM	2473	C	ALA				83.704	47.016	14.122		36.23		C
MOTA	2474	0			449		84.572	47.530	14.823		36.73		0
MOTA	2475	CB			449		83.951	46.741	11.646		34.97		C
ATOM	2476	N	SER	Α	450		82.406	47.262	14.277		34.72		N
MOTA	2477	CA	SER	А	450		81.914	48.166	15.310	1.00	34.31		C
MOTA	2478	C	SER	Α	450		82.313	47.717	16.714	1.00	34.50		С
ATOM	2479	0	SER	Α	450		82.868	48.501	17.493	1.00	31.24		0
MOTA	2480	CB	SER	A	450		80.387	48.279	15.235	1.00	33.37		C
ATOM	2481	QG	SER	A	450		79.991	49.068	14.130	1.00	33.43		0
ATOM	2482	N .	LEU	Α	451		82.043	46.450	17.026	1.00	34.30		N
ATOM	2483	CA			451		82.348	45.923	18.346	1.00	35.10		С
ATOM	2484	C	LEU				83.838	45.784	18.631	1.00	36.71		C
ATOM	2485	Ō	LEU				84.245	45.789	19.791		36.58		0
ATOM	2486	СВ	LEU				81.621	44.596	18.565		34.20		C
ATOM	2487		LEU				80.095	44.766	18.562		34.08		. C
ATOM	2488		LEU				79.423	43.457	18.926		32.06		C
											32.22		C
ATOM	2489		LEU				79.693	45.861	19.543				
ATOM	2490	N			452		84.655	45.665	17.588		37.71		N
MOTA	2491	CA			452		86.089	45.579	17.811		39.20		C
ATOM	2492	С			452		86.536	46.934	18.347		38.74		C
MOTA	2493	0			452		87.394	47.009	19.231		38.71		0
MOTA	2494	CB	ASN	A	452		86.853	45.263	16.523		40.36		С
MOTA	2495	CG.	ASN	Α	452		86.888	43.781	16.215		44.54		С
MOTA	2496	OD1	ASN	Α	452		86.761	42.940	17.113	1.00	46.29		0
MOTA	2497	ND2	ASN	Α	452		87.085	43.447	14.941	1.00	46.83		N
MOTA	2498	N	LYS	Α	453		85.949	48.001	17.812	1.00	37.17		N
MOTA	2499	CA			453		86.292	49.347	18.256	1.00	37.39		C
MOTA	2500	С			453 -		85.809	49.571	19.685		35.35		С
ATOM	2501	0			453		86.501	50.197	20.481		35.05		0
ATOM	2502	CB			453		85.700	50.395	17.303		38.34		C
ATOM	2503	CG			453		86.488	50.492	15.995		42.57		C
71011	2003	CG	מונג		- <del>1</del> - J		50.400	30.432	10.000	1.00	12.57		_

MOTA	2504	CD	LYS			85.717	51.157	14.858		44.00		С
MOTA	2505	CE	LYS			85.478	52.635	15.094	1.00	45.69		С
MOTA	2506	NZ	LYS			84.699	53.222	13.962	1.00	46.71		N
MOTA	2507	N	VAL			84.631	49.048	20.008	1.00	32.74		N
MOTA	2508	CA	VAL			84.093	49.188	21.352		31.66	•	С
MOTA	2509	C	LAV			85.019	48.455	22.328	1.00	32.27		С
MOTA	2510	0	VAL			85.418	49.007	23.358	1.00	30.47		0
MOTA	2511	CB	JAV	Α	454	82.663	48.597	21.455	1.00	31.71		С
MOTA	2512		LAV			82.225	48.527	22.920	1.00	30.29		С
MOTA	2513	CG2	LAV	Α	454	81.680	49.459	20.651	1.00	30.64		С
MOTA	2514	N	LYS	Α	455	85.365	47.216	21.989	1.00	32.48		N
MOTA	2515	CA	LYS	Α	455	86.245	46.402	22.828	1.00	34.26		С
MOTA	2516	C	LYS	Α	455	87.589	47.081	23.053	1.00	34.74		C
MOTA	2517	0	LYS	A	455	88.123	47.081	24.162	1.00	34.39		0
MOTA	2518	CB	LYS	Α	455	86.483	45.035	22.182	1.00	34.75		С
MOTA	2519	CG	LYS	Α	455	85.336	44.055	22.297	1.00	35.60		C
MOTA	2520	CD	LYS	Α	455	85.607	42.860	21.395	1.00	38.09		C
MOTA	2521	CE	LYS	Α	455	84.529	41.811	21.508	1.00	41.48		C
MOTA	2522	NZ	LYS	Α	455	84.809	40.638	20.627	1.00	41.09		N
MOTA	2523	N	SER	A	456	88.140	47.652	21.989	1.00	35.13		N
ATOM	2524	CA	SER	Α	456	89.421	48.327	22.090	1.00	36.02		С
MOTA	2525	С	SER	Α	456	89.313	49.533	23.031		35.16		C
MOTA	2526	0	SER	Α	456	90.171	49.744	23.890	1:00	33.17		0
ATOM	2527	CB	SER			89.888	48.764	20.702	1.00	36.46		С
ATOM	2528	OG	SER			91.172	49.341	20.779		39.49		0
MOTA	2529	N	THR			88.254	50.320	22.875		33.64		N
MOTA	2530	CA	THR			88.056	51.478	23.734		33.01		C
ATOM	2531	C	THR			87.863	51.029	25.182		32.03		Ċ
MOTA	2532	0	THR			88.352	51.672	26.108		32.59		0
ATOM	2533	СВ	THR			86.835	52.297	23.286		32.27		C
ATOM	2534	OG1			457	87.050	52.756	21.949		34.93		o
ATOM	2535	CG2	THR			86.624	53.497	24.193		29.23		Ċ
MOTA	2536	N	MET			87.150	49.926	25.379		31.95		N
ATOM	2537	CA	MET			86.925	49.419	26.723		30.89		C
ATOM	2538	C	MET			88.256	49.114	27.407		32.55		C
ATOM	2539	0	MET			88.426	49.391	28.598		31.39		0
ATOM	2540	СВ	MET			86.031	48.179	26.683		30.61		c
MOTA	2541	CG	MET			84.548	48.518	26.564		28.50		C
ATOM	2542	SD	MET			83.488	47.100	26.262		29.80		S
ATOM	2543	CE	MET			83.570	46.223	27.839		27.13		C
ATOM	2544	N	CYS			89.211	48.568	26.660		32.81		N
ATOM	2545	CA	CYS			90.508	48.281	27.257		34.73		C.
ATOM	2546	C	CYS			91.260	49.572	27.583		34.20		C
ATOM	2547	0	CYS			91.998	49.620	28.566		33.88		0
ATOM	2548	CB	CYS			91.347	47.380	26.350		36.62		C
ATOM	2549	SG	CYS			90.944	45.616	26.569		40.92		s
ATOM	2550	N	ASN			91.075	50.610	26.766		32.61		N
ATOM	2551	CA	ASN			91.721	51.892	27.034		32.54	•	C
ATOM	2552	C	ASN			91.176	52.381	28.368		31.81		C
ATOM	2553		ASN			91.853	53.091					
ATOM	2554	O . CB	ASN			91.853	52.947	29.098 25.976		32.53 33.21		. O
ATOM	2555	CG	ASN					24.646				
ATOM	2556		ASN			92.034	52.693	•		35.78		C
						91.356	52.543	23.633		36.50		0
ATOM	2557		ASN			93.365	52.648	24.634		34.40		N
ATOM	2558	N .	CYS			89.932	52.010	28.668		31.68		N
ATOM	2559	CA	CYS			89.285	52.423	29.907		31.03		C
ATOM	2560	С	CYS	А	401	89.515	51.437	31.053	1.00	31.06		С

ATOM	2561	0	CYS	A	461	89.005	51.630	32.146	1.00 32.13			0
MOTA	2562	CB	CYS	Α	461	87.777	52.617	29.675	1.00 32.30			C
MOTA	2563	SG	CYS	А	461	87.364	53.913	28.455	1.00 34.10			S
MOTA	2564	N	GLY	Α	462	90.281	50.381	30.795	1.00 31.97			N
MOTA	2565	CA	GLY	Α	462	90.569	49.393	31.822	1.00 31.72			C
MOTA	2566	C	GLY	А	462	89.412	48.464	32.149	1.00 32.82			C
ATOM	2567	0	GLY	Α	462	89.277	47.995	33.282	1.00 32.24			0
MOTA	2568	N	ALA	А	463	88.588	48.171	31.151	1.00 31.78			N
MOTA	2569	CA	ALA	Α	463	87.427	47.320	31.362	1.00 31.54			С
MOTA	2570	C	ALA	Α	463	87.420	46.075	30.484	1.00 32.00			С
ATOM	2571	0	ALA	Α	463	87.657	46.150	29.278	1.00 31.09			0
ATOM	2572	CB	ALA	Α	463	86.160	48.132	31.126	1.00 30.25	•		С
ATOM	2573	N	LEU	Α	464	87.152	44.928	31.102	1.00 32.25			N
MOTA	2574	CA	LEU	Α	464	87.095	43.661	30.377	1.00 33.90			C
MOTA	2575	C.	LEU	À	464	85.652	43.241	30.158	1.00 32.84			C
MOTA	2576	0	LEU	A	464	85.380	42.324	29.386	1.00 34.74			0
MOTA	2577	CB			464	87.829	42.550	31.144	1.00 34.92			C
MOTA	2578	CG			464	89.345	42.457	30.945	1.00 36.98			C
MOTA	2579	CD1			464	89.906	41.276	31.739	1.00 38.71			C
ATOM	2580	CD2	LEU		•	89.647	42.278	29.470	1.00 37.33			C
MOTA	2581	N			465	84.732	43.906	30.850	1.00 31.76			N
MOTA	2582	CA			465	83.312	43.602	30.734	1.00 30.63			C
MOTA	2583	C			465	82.499	44.887	30.760	1.00 31.08			C
ATOM	2584	0			465	83.005	45.953	31.122	1.00 29.95			0
MOTA	2585	CB			465	82.835	42.718	31.891	1.00 31.43	·		C
MOTA	2586	OG1			465	82.906	43.464	33.110	1.00 32.51			Ō
ATOM	2587	CG2			465	83.710	41.464	32.010	1.00 30.28			Ċ
ATOM	2588	N			466	81.234	44.791	30.377	1.00 29.59			N
ATOM	2589	CA			466	80.386	45.965	30.376	1.00 28.97			C
ATOM	2590	C			466	80.180	46.491	31.797	1.00 28.90			C
ATOM	2591	0				80.254	47.696	32.034	1.00 29.22			o
ATOM	2592	CB			466	79.035	45.662	29.695	1.00 29.12			C
ATOM	2593	CG1	ILE			79.270	45.502	28.187	1.00 27.85			C
ATOM	2594	CG2	ILE			78.028	46.770	29.985	1.00 26.21			C
ATOM	2595	CD1				78.052	45.094	27.404	1.00 27.38			C
ATOM	2596	N			467	79.923	45.597	32.765	1.00 28.55		•	N
ATOM	2597	CA	PRO			79.733	46.105		1.00 28.14			C
MOTA	2598	С	PRO			80.986	46.813	34.642	1.00 29.41			C.
ATOM	2599	0	PRO			80.905	47.805	35.373	1.00 28.53			0
ATOM	2600	CB .	PRO			79.405	44.842	34.919	1.00 29.15			C
ATOM	2601	CG			467	78.676	43.992	33.890	1.00 28.98			C
ATOM	2602	CD	PRO	Α	467	79.588	44.163	32.688	1.00 27.09			C
ATOM	2603	N	GLN			82.151	46.314	34.253	1.00 30.32			N
ATOM	2604	CA			468	83.386	46.929	34.705	1.00 32.43			С
ATOM	2605	C	GLN			83.566	48.299	34.049	1.00 32.77			C
ATOM	2606	0	GLN			84.100	49.233	34.657	1.00 32.94			ō
ATOM	2607	CB	GLN			84.561	46.006	34.390	1.00 34.93			C
MOTA	2608	CG	GLN			85.869	46.461	34.969	1.00 36.80			C
ATOM	2609	CD	GLN			86.912	45.364	34.940	1.00 37.36			C
ATOM	2610	OE1	GLN			87.016	44.611	33.971	1.00 33.81			0
ATOM	2611	NE2	GLN			87.703	45.281	36.000	1.00 38.34			N
ATOM	2612	N	LEU			83.106	48.418	32.808	1.00 31.40			N
ATOM	2613	CA	LEU			83.191	49.672	32.082	1.00 30.05		•	C
MOTA	2614	С	LEU			82.263	50.700	32.729	1.00 29.95			C
MOTA	2615	0	LEU			82.628	51.862	32.899	1.00 29.45			ō
ATOM	2616	CB	LEU			82.780	49.471	30.620	1.00 30.63			C
ATOM	2617	CG	LEU			82.579	50.765	29.819	1.00 32.08			C
									<del>-</del>			-

ATOM	2618	CD1	LEU	Α	469	83.925	51.423	29.568	1.00 29.55		С
ATOM	2619	CD2	LEU	Α	469	81.882	50.454	28.493	1.00 32.46		С
ATOM	2620	N	${\tt GLN}$	Α	470	81.062	50.267	33.092	1.00 29.40		N
ATOM	2621	CA	GLN	Α	470	80.089	51.169	33.697	1.00 31.46		C
MOTA	2622	C	${\tt GLN}$	Α	470	80.599	51.680	35.039	1.00 33.28		C
MOTA	2623	0	GLN	Α	470 .	80.275	52.790	35.479	1.00 32.37		0
MOTA	2624	CB	GLN	Α	470 .	78.748	50.444	33.859	1.00 31.66		C
MOTA	2625	CG	GLN	Α	470	78.209	49.929	32.515	1.00 32.34		C
MOTA	2626	CD	GLN	Α	470	76.891	49.192	32.633	1.00 33.38		С
MOTA	2627	OE1	GLN	Α	470	76.671	48.454	33.585	1.00 34.59		0
MOTA	2628	NE2	GLN	Α	470	76.017	49.375	31.652	1.00 31.58		N
ATOM	2629	N	SER	Α	471	81.435	50.870	35.668	1.00 33.02		N
MOTA	2630	CA	SER	Α	471	81.997	51.222	36.955	1.00 34.85		С
ATOM	2631	C	SER	Α	471	83.239	52.119	36.863	1.00 33.52		С
ATOM	2632	, 0	SER	Α	471 .	83.374	53.070	37.625	1.00 34.04		0
ATOM	2633	CB	SER	Α	471	82.329	49.934	37.722	1.00 34.20		С
ATOM	2634	OG	SER	Α	471	82.985	50.221	38.940	1.00 40.00		. 0
ATOM	2635	N	LYS	Α	472	84.121	51.837	35.910	1.00 33.54		N
ATOM	2636	CA	LYS	Α	472	85.375	52.582	35.774	1.00 33.02		·C
ATOM	2637	C	LYS	Α	472	85.437	53.746	34.784	1.00 32.17		C
MOTA	2638	0	LYS	Α	472	86.312	54.599	34.904	1.00 32.35	•	0
ATOM	2639	CB	LYS			86.505	51.605	35.431	1.00 33.39		С
ATOM	2640	CG	LYS	Α	472	86.599	50.420	36.374	1.00 35.66		С
ATOM	2641.	CD			472.	87.597	49.369	35.885	1.00 37.76		C
MOTA	2642	CE	LYS	Α	472	89.036	49.761	36.185	1.00 40.51		С
MOTA	2643	NZ	LYS	Α	472	90.004	48.705	35.750	1.00 41.85		N
MOTA	2644	N	ALA	Α	473	84.538	53.782	33.804	1.00 30.79		N
MOTA	2645	CA	ALA	Α	473	84.563	54.849	32.806	1.00 30.86		C
ATOM	2646	С	ALA	Α	473	84.644	56.263	33.382	1.00 30.77		С
MOTA	2647	0	ALA	Α	473	83.971	56.599	34.358	1.00 31.90	•	0
ATOM	2648	CB	ALA			83.343	54.738	31.882	1.00 30.21		С
MOTA	2649	N			474	85.491	57.077	32.762	1.00 31.21		N
MOTA	2650	CA			474	85.685	58.476	33.136	1.00 31.60		C
ATOM	2651	С			474	85.118	59.211	31.930	1.00 32.45		C
ATOM	2652	0			474	85.681	59.165	30.829	1.00 30.42		0
ATOM	2653	CB			474	87.175	58.769	33.326	1.00 30.92		С
ATOM	2654	CG			474	87.773	58.010	34.520	1.00 31.60		С
ATOM	2655	CD	LYS			89.251	57.668	34.302	1.00 32.08		С
ATOM	2656	CE	LYS			90.125	58.906	34.302	1.00 32.99		С
MOTA	2657	NZ	LYS			91.550	58.543	34.039	1.00 33.32		N
ATOM	2658	N			475	83.990	59.875	32.146	1.00 32.69		N
ATOM	2659	CA				83.285	60.546	31.066	1.00 33.22		С
ATOM	2660	C			475	83.237	62.056	31.203	1.00 32.93		С
ATOM	2661	0			475	82.713	62.581	32.183	1.00 33.43		0
ATOM	2662	CB			475	81.848	59.991	30.977	1.00 33.86		C
ATOM	2663		ILE			81.907	58.456	30.907	1.00 34.55		C
ATOM	2664		ILE			81.128	60.569	29.758	1.00 34.88		C
MOTA	2665		ILE			80.562	57.756	31.036	1.00 33.21		C
ATOM '	2666	N			476	83.786	62.751	30.212	1.00 32.44		N
ATOM	2667	CA			476.	83.792	64.206	30.239	1.00 31.82		C
ATOM	2668	C			476	82.921	64.803	29.154	1.00 31.41		C
ATOM	2669	O			476	82.734	64.225	28.084	1.00 29.60		0
ATOM	2670	CB			476	85.212	64.803	30.054	1.00 31.71		C
MOTA	2671		THR			85.143	66.233	30.185	1.00 32.39		0
ATOM ATOM	2672		THR			85.770	64.464	28.665	1.00 28.14		C
ATOM	2673 2674	N CA				82.391	65.977	29.461	1.00 32.16	•	N
ATON	2674	CM	LEU	A	<b>4</b> //	81.569	66.737	20.542	1.00 34.25		С

ATOM	2675	C	LEU	A	477	82.595	67.593	27.787	1.00 34.56			С
MOTA	2676	Ο,	LEU	Α	477	83.646	67.907	28.345	1.00 32.54		•	0
MOTA	2677	CB	LEU	Α	477	80.622	67.621	29.357	1.00 35.42			С
ATOM '	2678	CG	LEU	Α	477	79.408	68.279	28.719	1.00 37.43			С
MOTA	2679	CD1	LEU	A	477	78.496	67.223	28.120	1.00 34.96			С
ATOM	2680	CD2	LEU	Α	477	78.667	69.082	29.798	1.00 39.05			С
MOTA	2681	N	VAL	Α	478	82.320	67.941	26.531	1.00 35.71			N
MOTA	2682	CA	VAL	Α	478	83.242	68.778	25.761	1.00 38.92			C
MOTA	2683	C	VAL	Α	478	82.573	70.119	25.463	1.00 41.05			С
MOTA	2684	0	VAL			81.359	70.187	25.298	1.00 40.84			0
MOTA	2685	СВ	VAL			83.659	68.111	24.428	1.00 39.90			С
ATOM .	2686	CG1				84.015	66.662	24.672	1.00 40.76			C
ATOM	2687	CG2				82.551	68.237	23.400	1.00 41.86			C
ATOM	2688	N			479	83.370	71.181	25.386	1.00 43.62			N
ATOM	2689	CA			479	82.849	72.525	25.147	1.00 47.07			C
ATOM	2690	C			479	82.082	72.745	23.854	1.00 50.19			Ċ
ATOM	2691	0			479	82.356	72.129	22.821	1.00 49.40	-		0
ATOM	2692	СВ			479	83.979	73.553	25.207	1.00 46.48			C
ATOM	2693	OG			479	84.904	73.327	24.160	1.00 46.18			0
ATOM	2694	N			.480	81.124	73.662	23.933	1.00 54.55			N
ATOM	2695	CA	SER			80.297	74.036	22.799	1.00 59.07			C
ATOM	2696	C			480	81.192	74.534	21.668	1.00 61.48			C
ATOM	2697	0			480	81.036	74.146	20.505	1.00 61.36			0
ATOM	2698	CB	SER			79.327	75.143	23.224	1.00 59.36			C
MOTA	2699	OG	SER			78.625	75.669	22.113	1.00 62.01			0
ATOM	2700	N	VAL			82.145	75.382	22.040	1.00 64.75			N
ATOM	2701	CA	VAL			83.088	75.982	21.104	1.00 67.50			C
ATOM	2702	C	VAL			84.162	75.015	20.611	1.00 69.03			C
ATOM	2702	0	VAL			85.113	75.432	19.949	1.00 69.98			0
ATOM	2704	CB	VAL			83.804	77.179	21.753	1.00 67.66			C
ATOM	2705	CG1				84.155	78.211	20.693	1.00 67.66			C
ATOM	2706		VAL			82.935	77.775	22.841	1.00 67.94			C
		N			482							
ATOM ATOM	2707					84.016	73.731	20.922				N C
ATOM	2708	CA C			482	85.010	72.749	20.504	1.00 71.93			
ATOM	2709				482 482	84.445	71.675	19.590 18.841	1.00 73.15 1.00 73.05			С О
	2710	O			482	83.495	71.916					
ATOM	2711	CB				85.636	72.068	21.724	1.00 72.51			C
ATOM	2712	OG M			482	84.711	71,185	22.344	1.00 72.87			0
ATOM	2713	N			483	85.048	70.487	19.686	1.00 74.34			N
ATOM	2714	CA			483	84.698	69.305	18.899				C
MOTA	2715	C			483	85.510	69.316	17.609	1.00 75.65			C
ATOM	2716	0			483	85.821	68.263	17.049	1.00 75.17			0
MOTA	2717	CB			483	83.189	69.254	18.536	1.00 75.76			С
MOTA	2718		ILE			82.338	69.219	19.809	1.00 75.65			C
ATOM	2719		ILE			82.903	68.025	17.680	1.00 75.47			C
ATOM	2720		ILE			80.852	69.350	19.554	1.00 74.79			C
ATOM	2721	N	VAL			85.854	70.517	17.150	1.00 76.42			N
ATOM	2722	CA	VAL			86.630	70.686	15.924	1.00 77.07			C
ATOM .	2723	C	VAL			88.022	70.077	16.085	1.00 77.20			C
ATOM	2724	0	VAL			88.540	69.442	15.163	1.00 77.05			0
ATOM	2725	CB	VAL			86.773	72.186	15.549	1.00 77.33			C
MOTA	2726		VAL			87.463	72.322	14.193	1.00 77.06			C
ATOM	2727		VAL			85.401	72.853	15.521	1.00 76.24			C
ATOM	2728	N			485	88.620	70.272	17.259	1.00 77.14			N
ATOM	2729	CA	GLU			89.948	69.733	17.545	1.00 77.36			C
ATOM	2730	С			485	89.935	68.210	17.439	1.00 77.78			C
ATOM	2731	0	GLU	A	485	90.907	67.599	16.991	1.00 77.16			0

MOTA	2732	CB	GLU	A	485	9	0.398	70.127	18.957	1.00	76.63		С
MOTA	2733	CG			485	9:	1.730	69.499	19.372	1.00	76.08		С
ATOM	2734	CD	GLU	A	485	92	2.030	69.654	20.854	1.00	75.36		С
MOTA	2735	OE1	GLU	A	485	9:	1.261	69.135	21.687	1.00	75.07		0
ATOM	2736	OE2	GLU	A	485	9:	3.041	70.294	21.190	1.00	75.66		0
ATOM	2737	N	GLY	A	486	88	8.824	67.610	17.861	1.00	78.37		N
MOTA	2738	CA	GLY	Α	486	88	8.682	66.165	17.831	1.00	79.06		C
MOTA	2739	С	$\operatorname{GLY}$	Α	486	88	8.873.	65.533	16.466	1.00	79.40		C
ATOM	2740	. 0	GLY	A	486	89	9.530	64.499	16.348	1.00	79.68		0
MOTA	2741	N	$\mathtt{GLY}$	Α	487	88	8.295	66.145	15.435	1.00	79.72		N
MOTA	2742	CA	$\mathtt{GLY}$	Α	487	88	8.428	65.611	14.091	1.00	79.91		C
MOTA	2743	С	GLY	A	487	. 89	9.646	66.164	13.376	1.00	80.25		C
MOTA	2744	0	$\operatorname{GLY}$	Α	487	9(	0.467	66.857	13.982	1.00	80.14		0
MOTA	2745	N	ALA	Α	488	89	9.773	65.854	12.088	1.00	80.34		N
MOTA	2746	CA	ALA	A	488	90	0.896	66.341	11.292	1.00	80.30		С
MOTA	2747	C	ALA	Α	488	· 90	0.694	67.833	11.037	1.00	80.42		. C
MOTA	2748	0	ALA	Α	488	89	9.584	68.272	10.730	1.00	79.93		0
MOTA	2749	CB	ALA	Α	488	90	0.972	65.584	9.969	1.00	79.95		С
MOTA	2750	N	HIS	Α	489	9:	1.763	68.612	11.165		80.61		N
MOTA	2751	CA	HIS	Α	489	91	1.661	70.052	10.957	1.00	81.04		C
ATOM	2752	C	HIS	Α	489	92	2.937	70.687	10.424	1.00	81.07		C
MOTA	2753	0	HIS	Α	489		1.046	70.253	10.742		80.28		0
MOTA	2754	CB	HIS	Α	489	91	1.271	70.743	12.266		81.48		C
MOTA	2755	CG	HIS	A	489	92	2.196	70.442	13.405		81.91		C
MOTA	2756	ND1	HIS	Α	489	92	2.241	69.210	14.020		81.93		N
ATOM	2757	CD2	HIS	Α	489		3.121	71.209	14.030		81.89		C
MOTA	2758	CE1	HIS	Α	489		3.153	69.231	14.976		81.92		C
MOTA	2759		HIS				3.702	70.432	15.002		81.66		N
MOTA	2760	N			490	92	2.758	71.727	9.614		81.38		N
MOTA	2761	CA			490		3.870	72.467	9.027		81.57		C
MOTA	2762	C	ASP	Α	490		1.730	71.605	8.111		81.88		Ċ
MOTA	2763	0	ASP	Α	490	95	5.940	71.810	7.997		81.99		0
MOTA	2764	CB	ASP	A	490	94	1.721	73.079	10.141		81.37		C
MOTA	2765	CG	ASP	Α	490	93	3.915	73.990	11.046		81.51		C
MOTA	2766	OD1	ASP	Α	490		3.484	75.069	10.579		81.11		ō
ATOM	2767	OD2	ASP	Α	490	93	3.701	73.622	12.220		81.49		0
MOTA	2768	N	VAL	Α	491	94	1.093	70.638	7.462		81.98		N
MOTA	2769	CA	VAL	A	491	94	1.779	69.748	6.537		82.24		C
MOTA	2770	С			491	93	3.841	69.392	5.390		82.41		C
MOTA	2771	0	VAL	Α	491		2.621	69.331	5.566		81.92		0
ATOM	2772	CB					5 252	68.440	7.231	_	82.15		C
MOTA	2773	CG1	VAL	Α	491		5.314	68.755	8.273		82.08		C
MOTA	2774		VAL				1.069	67.727	7.873		82.18		C
ATOM	2775	N			492		1.419	69.169	4.215		82.73		N
ATOM	2776	CA			492		3.651	68.816	3.029		83.15		C
ATOM	2777	C	ILE	Α	492		3.731	67.309	2.792		83.71		C
ATOM	2778	0			492		.558	66.887	1.954		84.19		0
MOTA	2779	CB			492		.180	69.565	1.782		83.08		Ċ
MOTA	2780	CG1	ILE				1.136	71.075	2.032		82.87		C
MOTA	2781		ILE				3.342	69.211	0.560		82.77		C
ATOM	2782		ILE				1.640	71.911	0.874		83.43		C
TER	2783				492				- · ·	•			_
HETATM		NA	NA		901	65	.965	62.918	15.945	1.00	69.25		NA
HETATM		K		Α	900		.585	53.172	29.328		36.10		K
HETATM		P	RVP		602		7.957	55.327	15.029		40.98		P
HETATM		01P			602		7.605	55.290	13.581		40.82		Ô
HETATM		02P			602		3.778	54.118	15.349		40.06		0
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HETATM	2789	03 P	RVP	602	68.738	56.618	15.412	1.00 40.73		0
HETATM	2790	05*	RVP	602	66.712	55.356	16.019	1.00 39.48		0
HETATM	2791	C5*	RVP	602	65.743	54.315	15.953	1.00 38.43		С
HETATM	2792	C4*	RVP	602	64.678	54.509	16.989	1.00 38.00		C
HETATM	2793	04*	RVP	602	63.938	55.721	16.576	1.00 38.49		0
HETATM	2794	C3*	RVP	602	63.577	53.475	17.169	1.00 36.61		С
HETATM	2795	03*	ŔVP	602	63.978	52.319	17.881	1.00 35.40		0
HETATM	2796	C2*	RVP	602	62.504	54.269	17.841	1.00 36.75		C
HETATM	2797	02*	RVP	602	62.653	54.352	19.240	1.00 36.68		0
HETATM	2798	C1*	RVP	602	62.606	55.609	17.106	1.00 38.31		С
HETATM	2799	N9	RVP	602	61.637	55.746	15.950	1.00 40.51		N
HETATM	2800	C8	RVP	602	61.076	54.833	15.070	1.00 40.32		C
HETATM	2801	N7	RVP	602	60.285	55.383	14.214	1.00 40.61		N
HETATM	2802	C5	RVP	602	60.285	56.713	14.493	1.00 41.77		C
HETATM	2803	C6	RVP	602	59.586	57.820	13.858	1.00 41.63		С
HETATM	2804	06	RVP	602	58.824	57.752	12.898	1.00 40.85		0
HETATM	2805	N1	RVP	602	59.848	59.109	14.451	1.00 42.44		N
HETATM	2806	N4	RVP	602	61.119	56.976	15.575	1.00 41.17		N
HETATM	2807	C1	MOA	600	60.515	58.824	19.697	0.50 46.30		C
HETATM	2808	C2	MOA	600	55.761	57.322	16.893			C
HETATM	2809 ·	C3-	MOA	600	54.536	56.866	16.570	0.50 50.25	•	·C
HETATM	2810	C4	MOA	600	53.366	57.590	17.224	0.50 51.18		C
HETATM	2811	C5	MOA	600	52.702	56.677	18.266	0.50 52.05		C
HETATM	2812	C6	MOA	600	53.320	56.768	19.656	0.50 52.48		C
HETATM	2813	C7	MOA	600	59.541	53.995	20.040	0.50 45.22		C
HETATM	2814	C8	MOA	600	56.392	53.973	18.496	0.50 45.61		C
HETATM	2815	C9	MOA	600 .	54.279	55.668	15.641	0.50 50.49		Ċ
HETATM	2816	C10	MOA	600	60.943	56.779	20.807	0.50 45.42		C
HETATM	2817	C11	MOA	600	59.925	56.532	19.711	0.50 45.86		C
HETATM	2818	C12	MOA	600.	59.265	55.296	19.328	0.50 45.51		C
HETATM	2819		MOA	600	58.321	55.359	18.230	0.50 45.35		Ċ
HETATM	2820	C14		600	58.073	56.626	17.563	0.50 46.27	,	C
HETATM	2821		MOA	600	58.756	57.824	17.978	0.50 45.96		. C
HETATM	2822	C16	MOA	600	59.679	57.745	19.060	0.50 46.34		C
HETATM	2823	C17	MOA	600	57.082	56.722	16.411	0.50 47.60		C
HETATM	2824	01	MOA	600	60.600	59.983	19.446	0.50 47.39		Ö
HETATM	2825	02	MOA	600	61.200	58.218	20.669	0.50 46.12		0
HETATM	2826	03	MOA	600	57.682	54.195	17.849	0.50 44.59		Ö
HETATM.	2827	04	MOA	600	58.494	59.017	17.318	0.50 45.53		Ö
HETATM	2828	05	MOA	600	53.045	57.763	20.364	0.50 53.35		Ö
HETATM	2829	06	MOA	600	54.072	55.841	20.036	0.50 50.72		0
HETATM	2830	Ο,	HOH	1	86.937	48.115	13.619	1.00 53.10		0
HETATM	2831	0	HOH	2	66.156	60.715	24.787	1.00 30.04		0
HETATM	2832	0	HOH	3	57.859	59.028	28.431	1.00 32.40		O
HETATM	2833	0	HOH	4	71.017	54.648	22.049	1.00 29.86		Ō
HETATM	2834	0	НОН	5	59.607	45.471	36.968	1.00 31.13		Ō
HETATM	2835	0	HOH	6	66.879		38.970	1.00 31.37		0
HETATM	2836	0	HOH	7	79.892	42.101	29.537	1.00 28.27		Ō
HETATM	2837	0	нон	8	75.265	45.936	32.827	1.00 34.43		Ō
HETATM	2838	0	HOH	9	56.912	79.011	34.524	1.00 32.22		Ō
HETATM	2839	0	НОН	10	71.224	53.547	14.238	1.00 33.27		Ö
HETATM	2840	0	HOH	11	87.551	55.794	31.268	1.00 29.17		o
HETATM	2841	0	HOH	12	78.951	48.244	37.321	1.00 38.69		Ö
HETATM	2842	0	НОН	13	76.535	44.032	31.071	1.00 33.29		o
HETATM	2843	0	нон	14	77.984	54.327	34.370	1.00 35.16		Ö
HETATM		0	НОН	15	84.500	53.321	21.118	1.00 31.74		o
HETATM	2845	Ο.	HOH	16	74.544	60.085	37.904	1.00 44.09		ō
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HETATM	2846	0	HOH	17	88.665	54.024	33.427	1.00	31.82			0
HETATM	2847	0	HOH	18	64.790	41.466	7.903	1.00	37.49			0
HETATM	2848	0	HOH	19	73.871	57.655	36.239	1.00	31.87			0
HETATM	2849	0	HOH	20	58.900	51.481	22.980	1.00				0
HETATM	2850	0	HOH	21	64.317	56.651	20.399	1.00				0
HETATM	2851	0	HOH	22	65.490	36.877	34.840	1.00				0
HETATM		0	HOH	23	60.085	50.861	20.174	1.00				0
HETATM		0	HOH	24	76.358	52.869	36.274	1.00				0
HETATM		0	HOH	25	64.918	73.696	32.920	1.00				0
HETATM		0	HOH	26	56.665	77.507	37.267	1.00				0
HETATM		0	НОН	27	72.867	38.426	33.907	1.00				0
HETATM		0	НОН	28	72.686	61.731	21.624	1.00				0
HETATM		0	HOH	29	67.317	67.438	30.698	1.00				0
HETATM		0	НОН	30	49.555	44.437	21.119	1.00				0
HETATM		0	нон	31	70.551	33.609	27.633	1.00				0
HETATM		0	нон	32	76.699	41.425	32.331	1.00				0
HETATM		0	НОН	33	61.925	50.659	17.855	1.00				0
HETATM		0	НОН	34	62.610	38.767	34.074 38.879	1.00				0
HETATM		0	HOH	35	56.933	57.813	16.896		41.65	•	-	0
HETATM.		0	НОН	36	66.624	37.892	32.916	1.00	43.83			0
HETATM		0	HOH	37	69.286 53.353	68.051 51.944	38.099		36.77			0
HETATM		0	HOH	38	82.373	67.465	31.922		39.48			0
HETATM HETATM		0	нон нон	39 40	62.373	61.940	37.710		45.75			0
HETATM		0	HOH	41	60.077	59.723	30.997		46.18			0
HETATM		0	НОН	42	51.139	46.321	36.000		41.32			Ö
HETATM		0	НОН	43	59.604	51.735	16.489		35.27			Ö
HETATM		0	НОН	44	61.183	37.811	37.337		47.18			Ö
HETATM		0	нон	45	66.082	58.886	21.454		35.99			Ō
HETATM		0.	нон	46	66.187	63.971	21.615		43.24			Ö
HETATM		Ö	НОН	47	68.276	38.487	46.493		41.00			0
HETATM		Ö	НОН	48	73.810	65.033	30.854		44.46			0
HETATM		. 0		49	59.036	45.342	5.912	•	45.26			0
HETATM		0	НОН	50	58.693	35.801	27.026	1.00	42.44			0
HETATM		0	НОН	51	54.551	73.802	39.044	1.00	44.81			0
HETATM		0	НОН	52	59.942	51.276	9.798	1.00	38.47	•		0
HETATM		0	нон	53	75.437	38.984	31.295	1.00	41.54			0
HETATM	2883	0	HOH	54	56.511	41.592	37.450	1.00	50.73			0
HETATM	2884	0	HOH	55	55.967	71.689	16.393	1.00	42.82			. 0
HETATM	2885	0	HOH	56 ,	79.457	38.647	17.552	1.00	40.99			0
HETATM	2886	0	HOH	57	61.441	73.979	39.270	1.00	51.02			0
HETATM	2887	0	HOH	58	74.980	37.209	10.810		44.24			0
HETATM	2888	0	HOH	59	87.106	70.131	23.910		48.62			0
HETATM	2889	0	HOH	60	78.921	72.296	28.132		44.83.			0
HETATM		0	HOH	61	59.217	38.449	34.738		41.72			0
HETATM		0	HOH	62	62.392	64.439	35.307		38.87			0
HETATM		0	HOH	63	52.186	54.149	25.895		39.43			0
HETATM		0	HOH	64	91.884	51.151	35.362		47.95			0
HETATM		0	HOH	65	74.410	50.817	36.320		40.80			0
HETATM		0	HOH	66	75.694	70.804	31.847		45.76			0
HETATM		0	НОН	67	85.562	49.382	39.692		44.65			0
HETATM		0	НОН	68	50.848	31.856	16.493		47.42			0
HETATM		0	HOH	69	75.545	38.878	8.328		39.75			0
HETATM		0	HOH	70	72.184	67.522	32.127		41.79			0
HETATM		0	HOH	71	81.557	38.617	24.306		45.21			0
HETATM		0	HOH	72 73	82.150	63.522	21.264		45.28			0
HETATM	2902	0	нон	73	43.465	44.041	23.652	1.00	49.13			U

CONECT 2793 2792 2798

HETATM	2903	0	нон	74		65.282	64.106	36.024	1.00 42.80	)	0
HETATM	2904	0	нон	75		71.791	56.052	42.026	1.00 43.68	3	0
HETATM		Ο.	нон	76		70.611	32.750	38.320	1.00 50.18	3	0
HETATM			нон	77		65.746	28.372	26.829	1.00 51.32	2	0
HETATM			нон	78		46.316	49.216	27.478	1.00 49.98	3	0
HETATM			нон	79		66.218	28.865	15.007	1.00 49.39	9	0
HETATM			нон	80		45.899	41.751	13.150	1.00 50.3	5	0
HETATM			нон	81		67.812	59.668	38.963	1.00 53.98	3	0
HETATM			нон	82		67.783	69.548	38.244	1.00 50.7		0
HETATM			нон .	83		90.501	38.801	36.127	1.00 59.9	7	0
HETATM			нон	84		57.960	65.710	38.116	1.00 51.7		0
HETATM			НОН	85		48.770	54.414	37.079	1.00 51.5		0
			HOH	86		54.375	62.285	36.120	1.00 46.2		0
HETATM			НОН	87		60.479	39.480	6.892	1.00 48.3		Ō
HETATM						63.400	39.497	6.092	1.00 47.1		Ō
HETATM			HOH	88			43.115	8.014	1.00 55.1		Ö
HETATM			HOH	89		49.881	31.869	25.511	1.00 54.9		Ö
HETATM			HOH	90		48.799		40.277	1.00 57.1		Ö
HETATM			HOH	91		55.226	53.883		1.00 60.1		0
HETATM		_	нон	92	• -	84.876	42.783	10.201	1.00 50.1		0
HETATM		0	НОН	93		71.104	57.754	14.563			0
HETATM		0	HOH	94		81.517	55.070	13.507	1.00 56.5		0
HETATM		0	нон	95		69.719	68.895	35.986	1.00 50.0		
HETATM		0	HOH	96		48.667	81.714	40.322	1.00 56.6		0
HETATM		0	нон	97		79.523	40.573	32.112	1.00 41.2		0
HETATM	2927	0	HOH	98		50.394	78.735	40.269	1.00 61.0		0
HETATM		0	HOH	99		51.083	76.617	38.073	1.00 50.9		0
HETATM	2929	0	HOH	100		55.631	67.730	37.228	1.00 53.0		0
METATM	2930	0	HOH	101		63.222	78.551	34.890	1.00 55.3		0
HETATM	2931	0	нон	102		64.387	81.230	33.819	1.00 60.3		0
HETATM	2932	0	HOH	103		63.693	84.119	34.865	1.00 68.0		0
HETATM	2933	0	HOH	104		75.769	73.295	28.310	1.00 58.0		0
HETATM	2934	0	НОН	105		86.092	39.258	22.649	1.00 56.6	3	0
HETATM	2935	0	нон	106		62.744	55.138	1.577	1.00 43.5	1	0
HETATM	2936	0	HOH	107		74.933	63.024	19.409	1.00 54.2	2	0
HETATM	2937	0	HOH	108		69.789	45.377	46.398	1.00 46.1	. 8	0
HETATM		0	нон	109		74.595	39.323	37.886	1.00 62.4	6	0
HETATM	2939	0	нон	110		73.747	39.642	41.004	1.00 58.8	5	0
HETATM	2940	0	нон	111		72.104	32.691	30.025	1.00 49.5		0
HETATM	2941	0	НОН	112		78.793	70.848	25.397	1.00 58.1	.9	0
HETATM		0	нон	113		73.215	33.284	26.151	1.00 58.6	2	0
HETATM		0	нон	114		68.965		0.725		1	0
HETATM		0	нон .			96.151	46.659	27.632	1.00 52.0	19	0
HETATM		Ō	НОН	116		97.574	43.766	26.583	1.00 57.7	2	0
HETATM		Ö	нон	117		63.372		25.790	1.00 49.3	6	0
HETATM		Ö	нон	118		66.211	31.555		1.00 58.3	6	0
HETATM		0	нон	119		63.520					0 -
HETATM		Ö	нон	120		88.222	37.020			7	0
CONECT				120		••••	•				
CONECT											
CONECT			2788	2789	2790						
CONECT			2,00	2,00	2,50			•			
CONECT											
CONECT											
CONECT											
CONECT				2704							
CONECT											

```
CONECT 2794 2792 2795 2796
CONECT 2795 2794
CONECT 2796 2794 2797 2798
CONECT 2797 2796
CONECT 2798 2793 2796 2799
CONECT 2799 2798 2800 2806
CONECT 2800 2799 2801
CONECT 2801 2800 2802
CONECT 2802 2801 2803 2806
CONECT 2803 2802 2804 2805
CONECT 2804 2803
CONECT 2805 2803
CONECT 2806 2799 2802
CONECT 2807 2822 2824 2825
CONECT 2808 2809 2823
CONECT 2809 2808 2810 2815
CONECT 2810 2809 2811
CONECT 2811 2810 2812
CONECT 2812 2811 2828 2829
CONECT 2813 2818
CONECT 2814 2826
CONECT 2815 2809
CONECT 2816 2817 2825
CONECT 2817 2816 2818 2822
CONECT 2818 2813 2817 2819
CONECT 2819 2818 2820 2826
CONECT 2820 2819 2821 2823
CONECT 2821 2820 2822 2827
CONECT 2822 2807 2817 2821
CONECT 2823 2808 2820
CONECT 2824 2807
CONECT 2825 2807 2816
CONECT 2826 2814 2819
CONECT 2827 2821
CONECT 2828 2812
CONECT 2829 2812
MASTER 509 0 4 13
                                    0 0 6 2948 1 46
                                                                  39
                              18
END
Figure 8
P-UC 5430
Page 1
```

```
08-AUG-02
                                                                               1ME8
 HEADER
             OXIDOREDUCTASE
  TITLE
             INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
  TITLE
             2 TRITRICHOMONAS FOETUS WITH RVP BOUND
  COMPND MOL ID: 1;
  COMPND 2 MOLECULE: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE;
 COMPND 3 CHAIN: A;
COMPND 4 SYNONYM: IMP DEHYDROGENASE, IMPDH;
  COMPND 5 EC: 1.1.1.205;
  COMPND 6 ENGINEERED: YES
  SOURCE MOL ID: 1;
  SOURCE 2 ORGANISM SCIENTIFIC: TRITRICHOMONAS FOETUS;
  SOURCE 3 GENE: IMPDH;
 SOURCE 5 GENE: IMPDH,
SOURCE 4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE 5 EXPRESSION_SYSTEM_COMMON: BACTERIA;
SOURCE 6 EXPRESSION_SYSTEM_STRAIN: H712;
SOURCE 7 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
 SOURCE 8 EXPRESSION_SYSTEM_PLASMID: PBACE
JRNL AUTH G.L.PROSISE, J.WU, H.LUECKE

JRNL TITL CRYSTAL STRUCTURE OF T. FOETUS INOSINE

JRNL TITL 2 MONOPHOSPHATE DEHYDROGENASE IN COMPLEX WITH THE

JRNL TITL 3 INHIBITOR RIBAVIRIN REVEALS A CATALYSIS-DEPENDENT

JRNL TITL 4 ION BINDING SITE

JRNL REF TO BE PUBLISHED

JRNL REFN

REFN
JRNL
 REMARK 1
 REMARK 2
 REMARK 2 RESOLUTION. 1.90 ANGSTROMS.
 REMARK
 REMARK 3 REFINEMENT.
REMARK 3 PROGRAM
                              : CNS 1.1
 REMARK 3 AUTHORS
                              : BRUNGER, ADAMS, CLORE, DELANO, GROS, GROSSE-
 REMARK 3
                                : KUNSTLEVE, JIANG, KUSZEWSKI, NILGES, PANNU,
  REMARK 3
                                : READ, RICE, SIMONSON, WARREN
  REMARK 3
  REMARK 3 REFINEMENT TARGET : ENGH & HUBER
  REMARK 3
 REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS): 1.90
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS): 48.94
 REMARK 3 DATA CUTOFF
                                              (SIGMA(F)) : 0.000
 REMARK 3 OUTLIER CUTOFF HIGH (RMS(ABS(F))) : NULL
  REMARK 3 COMPLETENESS (WORKING+TEST) (%): 99.4
  REMARK 3 NUMBER OF REFLECTIONS
  REMARK 3
  REMARK 3 FIT TO DATA USED IN REFINEMENT.
 REMARK 3 CROSS-VALIDATION METHOD : THROUGH
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
                                                           : THROUGHOUT
           3 R VALUE
                              (WORKING SET) : 0.243
  REMARK
  REMARK 3 FREE R VALUE
                                                           : 0.258
  REMARK 3 FREE R VALUE TEST SET SIZE
                                                       (%): 5.000
  REMARK 3 FREE R VALUE TEST SET COUNT
                                                           : 2523
  REMARK 3 ESTIMATED ERROR OF FREE R VALUE : 0.005
  REMARK 3
  REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
```

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REMARK 3 TOTAL NUMBER OF BINS USED : 6
REMARK 3 BIN RESOLUTION RANGE HIGH (A): 1.90 REMARK 3 BIN RESOLUTION RANGE LOW (A): 2.02
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%): 99.90
REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 7832
REMARK 3 BIN R VALUE
                                  (WORKING SET) : 0.2820
REMARK 3 BIN FREE R VALUE : 0.295
REMARK 3 BIN FREE R VALUE TEST SET SIZE (%): 4.60
                                                : 0.2950
REMARK 3 BIN FREE R VALUE TEST SET COUNT : 378
REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.015
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 2727
REMARK 3 NUCLEIC ACID ATOMS
                                     : 0
REMARK 3 HETEROGEN ATOMS
                                     : 23
REMARK 3 SOLVENT ATOMS
                                     : 201
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2): 23.40
REMARK 3 MEAN B VALUE (OVERALL, A**2): 36.90
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2): 0.00000
REMARK 3 B22 (A**2) 0.00000
REMARK 3 B22 (A**2) : 0.00000
REMARK . 3 B33 (A**2) : 0.00000
REMARK 3 B12 (A**2) : 0.00000
REMARK 3 B13 (A**2) : 0.00000
REMARK 3 B23 (A**2): 0.00000
REMARK 3
REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM LUZZATI PLOT (A): 0.26
REMARK 3 ESD FROM SIGMAA
                                         (A) : 0.18
REMARK 3 LOW RESOLUTION CUTOFF
                                          (A) : 5.00
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT (A): 0.28
REMARK 3 ESD FROM C-V SIGMAA (A): 0.18
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS (A): 0.005
REMARK 3 BOND ANGLES
                                   (DEGREES) : 1.20
REMARK 3 DIHEDRAL ANGLES
                                   (DEGREES) : 22.70
REMARK 3 IMPROPER ANGLES (DEGREES): 0.71
REMARK 3
REMARK 3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                                  RMS SIGMA
REMARK 3 MAIN-CHAIN BOND
                                         (A**2) : 0.990 ; 1.500
                                         (A**2) : 1.660 ; 2.000
REMARK 3 MAIN-CHAIN ANGLE
REMARK 3 SIDE-CHAIN BOND
REMARK 3 SIDE-CHAIN ANGLE
REMARK 3
                                          (A**2) : 1.450 ; 2.000
                                   (A**2) : 2.260 ; 2.500
REMARK 3 BULK SOLVENT MODELING.
REMARK 3 METHOD USED : FLAT MODEL
REMARK 3 KSOL : 0.36
REMARK 3 BSOL
                        : 44.08
REMARK 3
REMARK 3 NCS MODEL : NULL
```

```
REMARK
         3
REMARK 3 NCS RESTRAINTS.
REMARK 3 NCS RESTRAINTS.

REMARK 3 GROUP 1 POSITIONAL (A): NULL; NULL

REMARK 3 GROUP 1 B-FACTOR (A**2): NULL; NULL
                                                    RMS SIGMA/WEIGHT
REMARK 3
REMARK 3 PARAMETER FILE 1 : PROTEIN REP. PARAM
REMARK 3 PARAMETER FILE 2 : PARAM.GNSOL
REMARK 3 PARAMETER FILE 3 : CIS_PEPTIDE.PARAM
REMARK 3 PARAMETER FILE 4 : RMP MPA.PAR
REMARK 3 PARAMETER FILE 5 : ION.PARAM
REMARK 3 PARAMETER FILE 6 : NULL
REMARK · 3 TOPOLOGY FILE 1 : PROTEIN.TOP
REMARK 3 TOPOLOGY FILE 2 : RMP.TOP
REMARK 3 TOPOLOGY FILE 3 : MPA.TOP
REMARK 3 TOPOLOGY FILE 4 : ION.TOP
REMARK 3 TOPOLOGY FILE 5 : TOPH.GNSOL
REMARK 3 TOPOLOGY FILE 6 : NULL
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: NULL
REMARK 4
REMARK 4 1ME8 COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 16-AUG-2002.
REMARK 100 THE RCSB ID CODE IS RCSB016850.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION REMARK 200 DATE OF DATA COLLECTION : 12-JUN-2001
REMARK 200 TEMPERATURE (KELVIN) : 100.0
REMARK 200 PH
                                     : 7.50
REMARK 200 NUMBER OF CRYSTALS USED
REMARK 200
REMARK 200 SYNCHROTRON
                                    (Y/N) : Y
REMARK 200 RADIATION SOURCE
                                           : SSRL
REMARK 200 BEAMLINE
                                           : 9-1
REMARK 200 X-RAY GENERATOR MODEL
                                           : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE
                                    (A) : 0.97
REMARK 200 MONOCHROMATOR
                                          : NULL
REMARK 200 OPTICS
                                          : NULL
REMARK 200
REMARK 200 DETECTOR TYPE
REMARK 200 DETECTOR TYPE : IMAGE PLATE REMARK 200 DETECTOR MANUFACTURER : MARRESEARCH
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE : SCALEPACK
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 50290 \,^{\smallfrown}
REMARK 200 RESOLUTION RANGE HIGH (A): 1.900
REMARK 200 RESOLUTION RANGE LOW
                                      (A) : 50.000
REMARK 200 REJECTION CRITERIA (SIGMA(I)): 0.000
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE
                                      (%): 99.9
REMARK 200 DATA REDUNDANCÝ
                                        : 10.000
REMARK 200 R MERGE
                                       (I) : 0.08000
REMARK 200 R SYM
                                      (I) : NULL
REMARK 200 <I/SIGMA(I) > FOR THE DATA SET : 33.8000
```

```
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 1.90
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 1.93
REMARK 200 COMPLETENESS FOR SHELL (%): 100.0
REMARK 200 DATA REDUNDANCY IN SHELL
                                           : NULL
                                     (I) : 0.60000
REMARK 200 R MERGE FOR SHELL
REMARK 200 R SYM FOR SHELL
                                      (I) : NULL
REMARK 200 <1/SIGMA(I) > FOR SHELL
                                           : 2.400
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: FOURIER SYNTHESIS
REMARK 200 SOFTWARE USED: CNS
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: SODIUM MALONATE, TRIS, 2-
REMARK 280 MERCAPTOETHANOL, EDTA, GLYCEROL
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 4 3 2
REMARK 290
REMARK 290
               SYMOP SYMMETRY
            NNNMMM OPERATOR
REMARK 290
REMARK 290
REMARK 290
                2555 -X,-Y,Z
              3555 -X,Y,-Z
4555 X,-Y,-Z
5555 Z,X,Y
6555 Z,-X,-Y
REMARK 290
REMARK 290
REMARK 290
REMARK 290
              7555
REMARK 290
                        -Z,-X,Y
               8555
REMARK 290
                        -Z,X,-Y
REMARK 290
                9555 Y,Z,X
REMARK 290
             10555 -Y,Z,-X
11555 Y,-Z,-X
REMARK 290
REMARK 290
               12555
                       -Y,-Z,X
             12555 -Y,-Z,X

13555 Y,X,-Z

14555 -Y,-X,-

15555 Y,-X,Z

16555 -Y,X,Z

17555 X,Z,-Y

18555 -X,Z,Y
REMARK 290
                       Y, X, -Z
                       -Y,-X,-Z
REMARK 290
REMARK 290
REMARK 290
REMARK 290
REMARK 290
REMARK 290
               19555 -X,-Z,-Y
REMARK 290
               20555 X,-Z,Y
               21555 Z,Y,-X
REMARK 290
               22555 Z,-Y,X
REMARK 290
               23555
REMARK 290
                        -Z,Y,X
            . 24555
REMARK 290
                       -Z,-Y,-X
REMARK 290
REMARK 290
              WHERE NNN -> OPERATOR NUMBER
REMARK 290
                MMM -> TRANSLATION VECTOR
REMARK 290
```

REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY REMARK 290 RELATED MOLECULES. REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 7 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY3 0.000000 0.000000 1 1.000000 0.00000 REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY3 0.000000 0.000000 2 1.000000 0.00000 REMARK 290 SMTRY1 3 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 3 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY3 3 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY1 4 1.000000 0.000000 -0.000000 0.00000 REMARK 290 SMTRY2 4 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY3 0.000000 0.000000 -1.000000 0.00000 REMARK 290 · 0.000000 SMTRY1 0.000000 1.000000 0.00000 REMARK 290 SMTRY2 5 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 5 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY1 0.000000 0.000000 6 1.000000 0.00000 REMARK 290 SMTRY2 -1.000000 0.000000 0.000000 0:00000 REMARK 290 SMTRY3 0.000000 -1.000000 6 0.000000 0.00000 REMARK 290 SMTRY1 7 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY2 7 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 7 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY1 0.000000 0.000000 -1.000000 8 0.00000 REMARK 290 SMTRY2 8 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 0.000000 -1.000000 8 0.000000 0.00000 REMARK 290 SMTRY1 9 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 9 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY3 9 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 10 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 10 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY3 10 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 11 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 11 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY3 11 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 12 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 12 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY3 12 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY1 13 0.00000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 1.000000 13 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 13 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY1 14 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 14 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 14 0.000000 0.000000 -1.000000 0.00000 REMARK 290 SMTRY1 15 0.000000 1.000000 0.000000 0.00000 REMARK 290 SMTRY2 15 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 15 0.000000 0.000000 0.00000 1.000000 REMARK 290 SMTRY1 16 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY2 16 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY3 16 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY1 17 1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 17 0.000000 0.000000 1.000000 0.00000 REMARK 290 SMTRY3 17 0.000000 -1.000000 0.000000 0.00000 REMARK 290 SMTRY1 18 -1.000000 0.000000 0.000000 0.00000 REMARK 290 SMTRY2 18 0.000000 0.000000 1.000000 0.00000

377

GLY A

REMARK 465

102

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SMTRY3 18 0.000000 1.000000 0.000000
                                                           0.00000
REMARK 290
           SMTRY1 19 -1.000000 0.000000 0.000000
                                                           0.00000
REMARK 290
           SMTRY2 19 0.000000 0.000000 -1.000000
                                                           0.00000
REMARK 290
            SMTRY3 19 0.000000 -1.000000 0.000000
                                                           0.00000
REMARK 290
                                                           0.00000
            SMTRY1 20 1.000000 0.000000 0.000000
REMARK 290
            SMTRY2 20 0.000000 0.000000 -1.000000
                                                           0.00000
REMARK 290
            SMTRY3 20 0.000000 1.000000 0.000000
REMARK 290
            SMTRY1 21 0.000000 0.000000 1.000000
                                                           0.00000
REMARK 290
           SMTRY2 21 0.000000 1.000000 0.000000
                                                           0.00000
REMARK 290
           SMTRY3 21 -1.000000 0.000000 0.000000
                                                           0.00000
REMARK 290
REMARK 290 SMTRY1 22 0.000000 0.000000 1.000000
                                                           0.00000
                                                           0.00000
           SMTRY2 22 0.000000 -1.000000 0.000000
REMARK 290
           SMTRY3 22 1.000000 0.000000 0.000000
                                                           0.00000
REMARK 290
           SMTRY1 23 0.000000 0:000000 -1.000000
                                                           0.00000
REMARK 290
REMARK 290 SMTRY2 23 0.000000 1.000000 0.000000 REMARK 290 SMTRY3 23 1.000000 0.000000 0.000000
                                                           0.00000
                                                           0.00000
REMARK 290 SMTRY1 24 0.000000 0.000000 -1.000000
                                                           0.00000
           SMTRY2 24 0.000000 -1.000000 0.000000
                                                           0.00000
REMARK 290
           SMTRY3 24 -1.000000 0.000000 0.000000
                                                           0.00000
REMARK 290
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300 '
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 1 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
                                                           0.00000
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000
                    1 0.000000 1.000000 0.000000
                                                           0.00000
            BIOMT2
REMARK 350
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000
                                                           0.00000
REMARK 350 BIOMT1 2 -1.000000 0.000000 0.000000
                                                         154.74500
REMARK 350 BIOMT2 2 0.000000 -1.000000 0.000000
                                                          154.74500
REMARK 350 BIOMT3 2 0.000000 0.000000 1.000000
                                                           0.00000
REMARK 350 BIOMT1 3 0.000000 1.000000 0.000000
                                                           0.00000
REMARK 350 BIOMT2 3 -1.000000 0.000000 0.000000
                                                          154.74500
           BIOMT3 3 0.000000 0.000000 1.000000
BIOMT1 4 0.000000 -1.000000 0.000000
                                                           0.00000
REMARK 350
                                                         154.74500
REMARK 350
REMARK 350 BIOMT2 4 1.000000 0.000000 0.000000
                                                          0.00000
                    4 0.000000 0.000000 1.000000
                                                           0.00000
           BIOMT3
REMARK 350
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465
             M RES C SSSEQI
           MET A 1
REMARK 465
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REMARK	465	PHE A	103
REMARK	465	VAL A	104
REMARK	465	VAL A	105
REMARK	465	SER A	106
REMARK	465	ASP A	107
REMARK	465	SER A	108
REMARK	465	ASN A	109
REMARK	465	VAL A	110
REMARK	465	LYS A	111
REMARK	465	PRO A	112
REMARK	465	ASP A	113
REMARK	465	GLN A	114
REMARK	465	THR A	115
REMARK	465	PHE A	116
REMARK	465	ALA A	117
REMARK	465	ASP A	118
REMARK	465	VAL A	119
REMARK	465	LEU A	120
REMARK	465	ALA A	121
REMARK	465	ILE A	122
REMARK	465	SER A	123
REMARK	465	GLN A	124
REMARK	465	ARG A	125
REMARK	465	THR A	126
REMARK	465	THR A	127
REMARK	465	HIS A	128
REMARK	465	ASN A	129
REMARK	465	THR A	130
REMARK		· VAL A	131
REMARK		ALA A	132
REMARK	465	VAL A	133
REMARK	465	THR A	134
REMARK	465	ASP A	135
REMARK	465	ASP A	136
REMARK	465	GLY A	137
REMARK	465	THR A	138
			139
REMARK		PRO A HIS A	140
REMARK REMARK		GLY A	141
	465	*	142
REMARK		VAL A LEU A	143
REMARK			
REMARK	465	LEU A	144 145
REMARK		GLY A	
REMARK		LEU A	.146
REMARK		VAL A	147
REMARK		THR A	148
		GLN A	149
REMARK		ARG A	150
REMARK		ASP A	151
REMARK	465	TYR A	152
REMARK		PRO A	153
REMARK		ILE A	154
REMARK		ASP A	155
REMARK		LEU A	156
REMARK		THR A	157
REMARK		GLN A	158
REMARK	465	THR A	159

REMARK	465	GLU	A	160
REMARK	465	THR	A .	161
REMARK	465	LYS	A	162
REMARK	465	VAL	A	163
REMARK	465	SER	A S	164
REMARK	465	ASF	A	165
REMARK	465	MET	A	166
REMARK	465	MET	A	167
REMARK	465	THE	A 9	168
REMARK	465	PRO	Α (	169
REMARK	465	PHE	A	170
REMARK	465	SEF	· A	171
REMARK	465	LYS	A S	172
REMARK	465	LEU	JA	173
REMARK	465	VAI	A	174
REMARK	465	THE	A S	175
REMARK	465	ALA	A	176
REMARK	465	HIS	a A	177
REMARK	465	GLÌ		178
REMARK	465	ASI		179
REMARK	465	THE		180
REMARK	465	LYS		181
REMARK	465	LEU		182
REMARK	465	SEI		183
REMARK	465	GL		184
REMARK	465	ALA		185
REMARK	465	ASI		186
REMARK	465	. LYS		187
REMARK	465	ILI		188
REMARK	465	ILI		189
REMARK	465	TRI		190
REMARK	465	GLU		191
	465	LYS		192
REMARK	465	LY		193
REMARK REMARK		LE		194
REMARK	465	ASI		195
	465			
REMARK	465	AL		196
REMARK		LE		197
REMARK		PRO		198
REMARK		IL		199
REMARK		IL		200
REMARK		ASI		201
REMARK		AS:		202
REMARK		AS:		203
REMARK		GL		204
REMARK		HI		205
REMARK		LE		206
REMARK		AR		207
REMARK		· TY		208
REMARK		IL		209
REMARK		VA		210
REMARK		PH		211
REMARK	•	AR		212
REMARK		LY		213
REMARK		AS		214
REMARK		TY		215
REMARK	465	AS	PΑ	216

```
REMARK 465
              ARG A
                       217
               SER A
                       218
REMARK 465
REMARK 465
               GLN A
                       219
REMARK 465
               VAL A
                       220 ·
REMARK 465
               CYS A
                       221
REMARK 465
               GLN A
                       417
REMARK 465
               ARG A
                       418
REMARK 465
               TYR A
                       419
               ASP A
REMARK 465
                       420
               LEU A
REMARK 465
                       421
REMARK 465
               GLY A
                       422
REMARK 465
               GLY A
                       423
               LYS A
REMARK 465
                       424
REMARK 465
               GLN A
                       425
REMARK 465
               LYS A
                       426
REMARK 465
                       427
               LEU A
REMARK 465
               SER A
                       428
REMARK 465
               PHE A
                       429
REMARK 465
               GLU A
                       430
               VAL A
REMARK 465
                       493
             LYS A
REMARK 465
                       494
REMARK 465
               ASP A
                       495
             ARG A
REMARK 465
                       496
REMARK 465
               ILE A
                       497
               ASN A
REMARK 465
                       498
               ASP A
REMARK 465
                       499
REMARK 465
               TYR A
                       500
REMARK 465
               HIS A
                       501
REMARK 465
               PRO A
                       502
REMARK 465
               LYS A
                       503
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
                                ATM2
REMARK 500 M RES CSSEQI ATM1
                                        ATM3
REMARK 500
                                        С
                                            ANGL. DEV. = -7.5 DEGREES
              GLY A 20
                          N
                                 CA
REMARK 500
              ILE A 27
                                 CA
                                        С
                                            ANGL. DEV. = -9.2 DEGREES
                          N
                                           ANGL. DEV. = 7.4 DEGREES
REMARK 500
              PRO A 53°
                                 CA
                                        C
                          N
              SER A 63
                                            ANGL. DEV. = 8.5 DEGREES
REMARK 500
                          N
                                 CA
                                        С
REMARK 500
              SER A 357
                                 CA
                                        С
                                            ANGL. DEV. = -7.3 DEGREES
                          N
REMARK 500
              LYS A 472
                          N
                             . _
                                 CA
                                        С
                                            ANGL. DEV. = 8.2 DEGREES
                                 CA - C
                                            ANGL. DEV. = -8.8 DEGREES
REMARK 500
              LYS A 474
                          N
                                 CA - C ANGL. DEV. = -8.6 DEGREES
REMARK 500
              LEU A 477
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1AK5
                              RELATED DB: PDB
REMARK 900 INOSINE MONOPHOSPHATE DEHYDROGENASE (IMPDH) FROM
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```
REMARK 900 TRITRICHOMONAS FOETUS
                           RELATED DB: PDB
REMARK 900 RELATED ID: 1ME7
REMARK 900 1ME7 CONTAINS THE SAME PROTEIN WITH RRP AND MOA BOUND
REMARK 900 RELATED ID: 1ME9 RELATED DB: PDB
REMARK 900 1ME9 CONTAINS THE SAME PROTEIN WITH IMP BOUND
REMARK 900 RELATED ID: 1MEH RELATED DB: PDB
REMARK 900 1MEH CONTAINS THE SAME PROTEIN WITH IMP AND MOA BOUND
REMARK 900 RELATED ID: 1MEI RELATED DB: PDB
                                             .
REMARK 900 1MEI CONTAINS THE SAME PROTEIN WITH XMP AND MYCOPHENOLIC
REMARK 900 ACID BOUND
REMARK 900 RELATED ID: 1MEW
                           RELATED DB: PDB
REMARK 900 1MEW CONTAINS THE SAME PROTEIN WITH XMP AND NAD BOUND
              1 503 SWS P50097 IMDH TRIFO
DBREF 1ME8 A
SEQADV 1ME8 CSO A 319 SWS P50097 CYS 319 MODIFIED RESIDUE
        1 A 503 MET ALA LYS TYR TYR ASN GLU PRO CYS HIS THR PHE ASN
SEORES
        2 A 503 GLU TYR LEU LEU ILE PRO GLY LEU SER THR VAL ASP CYS
SEQRES
        3 A 503 ILE PRO SER ASN VAL ASN LEU SER THR PRO LEU VAL LYS
SEORES
        4 A 503 PHE GLN LYS GLY GLN GLN SER GLU ILE ASN LEU LYS ILE
SEORES
        5 A 503 PRO LEU VAL SER ALA ILE MET GLN SER VAL SER GLY GLU
SEORES
        6 A 503 LYS MET ALA ILE ALA LEU ALA ARG GLU GLY GLY ILE SER
SEORES
        7 A 503 PHE ILE PHE GLY SER GLN SER ILE GLU SER GLN ALA ALA
SEORES
        8 A 503 MET VAL HIS ALA VAL LYS ASN PHE LYS ALA GLY PHE VAL
SEORES
             503 VAL SER ASP SER ASN VAL LYS PRO ASP GLN THR PHE ALA
       9 A
SEORES
SEQRES 10 A 503 ASP VAL LEU ALA ILE SER GLN ARG THR THR HIS ASN THR
SEQRES 11 A 503 VAL ALA VAL THR ASP ASP GLY THR PRO HIS GLY VAL LEU
       12 A 503 LEU GLY LEU VAL THR GLN ARG ASP TYR PRO ILE ASP LEU
SEORES
       13 A 503 THR GLN THR GLU THR LYS VAL SER ASP MET MET THR PRO
SEORES
       14 A 503 PHE SER LYS LEU VAL THR ALA HIS GLN ASP THR LYS LEU
SEQRES
       15 A 503 SER GLU ALA ASN LYS ILE ILE TRP GLU LYS LYS LEU ASN
SEORES
       16 A 503 ALA LEU PRO ILE ILE ASP ASP ASP GLN HIS LEU ARG TYR
SEORES
                 ILE VAL PHE ARG LYS ASP TYR ASP ARG SER GLN VAL CYS
SEORES
       17 A 503
       18 A 503 HIS ASN GLU LEU VAL ASP SER GLN LYS ARG TYR LEU VAL
SEORES
       19 A 503 GLY ALA GLY ILE ASN THR ARG ASP PHE ARG GLU ARG VAL
SEORES
       20 A 503 PRO ALA LEU VAL GLU ALA GLY ALA ASP VAL LEU CYS ILE
SEORES
       21 A 503 ASP SER SER ASP GLY PHE SER GLU TRP GLN LYS ILE THR
SEORES
             503 ILE GLY TRP ILE ARG GLU LYS TYR GLY ASP LYS VAL LYS
SEQRES
       22 A
             503 VAL GLY ALA GLY ASN ILE VAL ASP GLY GLU GLY PHE ARG
       23 A
SEORES
                  TYR LEU ALA ASP ALA GLY ALA ASP PHE ILE LYS ILE GLY
SEORES 24 A
             503
                  ILE GLY GLY GLY SER ILE CSO ILE THR ARG GLU GLN LYS
SEORES 25 A
             503
SEQRES 26 A 503 GLY ILE GLY ARG GLY GLN ALA THR ALA VAL ILE ASP VAL
SEQRES 27 A 503 VAL ALA GLU ARG ASN LYS TYR PHE GLU GLU THR GLY ILE
                  TYR ILE PRO VAL CYS SER ASP GLY GLY ILE VAL TYR ASP
SEORES
       28 A 503
                  TYR HIS MET THR LEU ALA LEU ALA MET GLY ALA ASP PHE
SEORES 29 A 503
SEQRES 30 A 503 ILE MET LEU GLY ARG TYR PHE ALA ARG PHE GLU GLU SER
       31 A 503 PRO THR ARG LYS VAL THR ILE ASN GLY SER VAL MET LYS
SEORES
       32 A 503 GLU TYR TRP GLY GLU GLY SER SER ARG ALA ARG ASN TRP
SEORES
       33 A 503 GLN ARG TYR ASP LEU GLY GLY LYS GLN LYS LEU SER PHE
SEORES
       34 A 503 GLU GLU GLY VAL ASP SER TYR VAL PRO TYR ALA GLY LYS
SEQRES
       35 A 503 LEU LYS ASP ASN VAL GLU ALA SER LEU ASN LYS VAL LYS
SEORES
       36 A 503 SER THR MET CYS ASN CYS GLY ALA LEU THR ILE PRO GLN
SEORES
       37 A 503 LEU GLN SER LYS ALA LYS ILE THR LEU VAL SER SER VAL
SEQRES
       38 A 503 SER ILE VAL GLU GLY GLY ALA HIS ASP VAL ILE VAL LYS
SEQRES
       39 A 503 ASP ARG ILE ASN ASP TYR HIS PRO LYS
SEQRES
MODRES 1ME8 CSO A 319 CYS S-HYDROXYCYSTEINE
                       7
HET
       CSO A 319
HET
       K 900
                       1
                      • 1
HET
        NA
              901
```

```
HET
       RVP
              602
                        21
           CSO S-HYDROXYCYSTEINE
HETNAM
          K POTASSÍUM ION
HETNAM
HETNAM
            NA SODIUM ION
           RVP RIBAVIRIN MONOPHOSPHATE
HETNAM
                    C3 H7 N1 O3 S1
FORMUL
         1
            CSO
              K
                    K1 1+
FORMUL
         2
FORMUL
         3
              NA
                    NA1 1+
            RVP
                    C8 H13 N4 O8 P1
FORMUL
          4
            HOH
                   *201(H2 O1)
FORMUL
         5
                        11
                             ASN A
                                     13
                                          5
HELIX
          1 . 1 THR A
3
              2 ILE A
                         27
                             VAL A
                                     31
                                          5
HELIX
          2
5
         3 `
                             GLU A
                                     74
HELIX
              3 GLY A
                         64
                                          1
11
                         85
                             ASN A
                                      98
HELIX
          4
              4 SER Ā
14
                                     254
HELIX
          5
              5 ASP A
                       242
                             GLY A
13
          6.
              6 SER A
                       267
                             GLY A
                                     282
HELIX
16
                                          5
          7
              7 ASP A
                       283
                             VAL A
                                     285
HELIX
3
HELIX
          8
              8 ASP A
                        294
                             GLY A
                                     305
12
HELIX
          9
              9 GLY A
                        330
                             GLY A
                                     350
                                          1
21
                                     373 1
HELIX
         10
             10 TYR A
                        363
                             MET A
11
                        381
                                     386
                                          1
HELIX
         11
             11 GLY A
                             ARG A
6
             12 SER A
                        410
                             ASN A
                                     4.15
HELIX
         12
6
                             CYS A
HELIX
         13
             13 LYS A
                        442
                                     461
                                          1
20
                       465
                             ALA A
                                     473
         14
             14 THR A
HELIX
9
SHEET
          1
              À 2 TYR A 15
                              LEU A 17
                                                                 LEU A
                                                                        16
                                                 THR A 476
                                                             N
              A 2 ILE A 475
                              LEU A 477 -1
                                             0
SHEET
          2
                                     3.6
              B 2 THR. A .35
                              PRO A
                                         0
SHEET
          1-
                                                                 THR A
                                                                        35
                              LEU A
                                     50 -1
                                                LEU A 50
              B 2 ASN A 49
                                             O
SHEET
          2
                                          0
                              GLN A 41
SHEET
          1
              C 2 PHE A 40
                                                                        40
                                                                 PHE A
                                                TYR A 352
                                                             N
              C 2 ILE A 351
                              TYR A 352 -1
                                             0
SHEET
          2
                                      56.
                                          0
              D 9 LEU A 54
                              SER A
SHEET
          1
                                                                        56
                                                ILE A 77
                                                             N
                                                                 SER A
                              ILE A
                                      80
                                             0
              D 9 ILE A
                          77
                                          1
SHEET
          2
                                                                 ILE A 80
                                                GLY A 237
                                                              N
                              ILE A 238
                                             0
              D 9 GLY A 235
 SHEET
          3
                                          1
                                                             N
                                                                 ILE A 238
                                                CYS A 259
                                             0
              D 9 VAL A 257
                               ILE A 260
                                          1
 SHEET
          4
                                                                 LEU A 258
                              ILE A 292
                                          1
                                             0
                                                 GLY A 288
                                                              Ν
          5
              D 9 VAL A 287
 SHEET
                                                                 ALA A 289
                                                 LYS A 310
                                                              Ν
                              ILE A 311
                                          1
                                             0
              D 9 PHE A 308
 SHEET
          6
                                                                 ILE A 311
                                             0
                                                 CYS A 356
                                                             N
                                          1
                              ASP A 358
 SHEET
          7
              D 9 VAL A 355
                                                                 SER A 357
                                                 MET A 379
                                                              N
                                             0
                              LEU A 380
                                          1
 SHEET
          8
              D 9 PHE A 377
                                                                 ILE A 378
                                             N
                                                 VAL A 55
                                                              0
          9
              D 9 LEU A 54
                              SER A 56
                                          1
 SHEET
              E 3 LYS A 394
                               ILE A 397
                                          0
 SHEET
          1
                                                MET A 402
                                                              N
                                                                 VAL: A 395
                                             0
              E 3 SER A 400
                               TRP A 406 -1
 SHEET
          2
                                                                 TYR A 405
                               PRO A 438 -1 O
                                                              N
              E 3 ASP A 434
                                                 SER A 435
          3
 SHEET
                           CYS A 459
          1 CYS A
                     26
 SSBOND
```

							•				
CISPEP	1 G	LY A	290 154.		ASN A	291 5 90 00	90.00	90.00 F	0.82 9 4 3 2	2	24
CRYST1		745 1.000			134.74	0.000000		0.00000			
ORIGX1						0.000000		0.00000			
ORIGX2		0.000			00000			0.00000			
ORIGX3		0.000			00000	1.000000					
SCALE1		0.006	462		00000	0.000000		0.00000			
SCALE2		0.000	000	0.0	006462	0.000000	,	0.00000			
SCALE3		0.000	000	0.0	00000	0.006462		0.00000			
ATOM	1	N	ALA	Α	2	55.144	74.892	36.640	1.00	29.93	
N											
ATOM	2	CA	ALA	Α	2	55.885	73.830	35.910	1.00	29.54	
C	_										
	3	С	ALA	Δ	2	57.177	73.489	36.647	1.00	30.30	
ATOM	3	C	АПА	Α.	2	3,.1,,	, , , , , ,		,		
C		•		70	2	57.618	74.234	37.525	1.00	29 88	
MOTA	4	0	ALA	Α .	2	57.616	14.234	37.323	1.00	22.00	
0								24 401	1 00	20 72	
MOTA	, 5	CB	ALA	A	2	56.201	74.301	34.491	1.00	29.72	
C					•						
ATOM	6	N	LYS	Α	3	57.771	72.357	36.289	1.00	29.86	
N											
ATOM	7	CA	LYS	Α -	3	59.015	71.919	36.904	1.00	30.69	
C											
ATOM	8	C	LYS	A	3 .	60.155	72.132	35.922	1.00	29.48	
C		•	<b>2</b> 10.		•	••••					
	9	0	LYS	7\	3	60.040	71.777	34.753	1.00	28.89	
MOTA	9	O	птэ	Α.	3	00.040	, , , ,				
0					2	50 043	70.434	37.275	1 00	33.07	
MOTA	10	CB	LYS	A	3	58.943	/0.434	31.213	1.00	33.07	
С					_			25 620	1 00:	27 75	
MOTA	11	CG	LYS	Α	3	60.304	69.840	37.628	1.00	37.75	
C								32 121			
MOTA	12	CD	LYS	A	3	60.240	68.344	37.872	1.00	41.04	
C											
MOTA	13	CE	LYS	Α	3	61.628	67.728	37.773	1.00	42.33	
C								•			
ATOM	14	NZ	LYS	A .	3	62.601	68.424	38.656	1.00	43.20	
N											
ATOM	15	N	TYR	Á	4 ·	61.252	72.704	36.407	1.00	28.93	
N	15				-						
	16	CA	TYR	<b>Z</b>	4	62.425	72.961	35.581	1.00	28.85	
ATOM	10	CA	IIK	Α	-		72.501				
C			mvn	70	4	62 620	72.167	36.109	1 00	29.60	
MOTA	17	. C	TYR	Α	4	63.620	12.107	30.105	1.00	23.00	
С		_		_		60 545	71 551	27 172	1 00	28.77	
MOTA	18	0	TYR	A	4	63.545	71.551	37.172	1.00	20.77	
0							0			00 00	
MOTA	19	CB	TYR	Α	4	62.732	74.463	35.571	1.00	28.38	
C											
MOTA	20	CG	TYR	Α	4	61.634	75.274	34.917	1.00	27.99	
C											
MOTA	21	CD1	TYR	Α	4	61.519	75.336	33.527	1.00	27.06	•
C											
MOTA	22	CD2	TYR	Α	4	60.684	75.946	35.686	1.00	28.17	
C	ب ب				-						
	23	CEI	TYR	20	4	60.479	76,050	32.919	1.00	27.85	
ATOM	23	CET	111		-	00.272				. –	
C	2.4	ana	יויי. מעליוני	- 7\	4	59.643	76 662	35.087	1,00	27.52	
ATOM	24	CB2	TYR	. д	#	JJ.043	,0.002	55.007		<b></b>	
C											

ATOM C		25	CZ	TYR	A	4	59.547	76.708	33.707	1.00	27.20
ATOM O		26	ОН	TYR	A	4	58.512	77.400	33.115	1.00	27.38
ATOM N		27	N	TYR	A	5	64.714	72.173	35.359	1.00	30.38
ATOM C		28	CA	TYR	A	5 .	65.909	71.436	35.756	1.00	31.23
ATOM C		29	С	TYR	A	5	67.109	72.364	35.895 ,	1.00	32.36
ATOM O		30	0	TYR	A	5	67.143	73.440	35.300	1.00	31.65
ATOM C		31	CB	TYR	A	5	66.204	70.330	34.739	1.00	31.26
ATOM C		32	CG	TYR	A	5, . ,	65.063	69.349	34.584	1.00	31.28
ATOM C		33	CD1	TYR	A	5	63.906	69.702	33.891	1.00	30.79
ATOM C		34	CD2	TYR	A	5	65.116	68.085	35.179	1.00	31.65
ATOM C		35	CE1	TYR	A	5	62.824	68.826	33.794	1.00	30.64
ATOM C		36 .	CE2	TYR	A	5	64.039	67.199	35.088	1.00	30.49
ATOM C		37	CZ	TYR	A	5	62.897	67.579	34.395	1.00	31.03
ATOM O	•	38	ОН	TYR	A	5	61.817	66.725	34.313	1.00	29.28
ATOM N		39	N	ASN	A	6	68.090	71.942	36.687	1.00	33.08
ATOM		40	CA	ASN	A	6	69.285	72.744	36.925	1.00	34.41
C ATOM C		41	С	ASN	Α	6 ,	70.250	72.779	35.744	1.00	34.13
ATOM O		42	0 .	ASN	A	6	70.971	73.758	35.556	1.00	34.71
ATOM C		43	СВ	ASN	A	6	70:009	72.226	38.171	1.00	37,.70
ATOM		44	CG	ASN	A	6	69.207	72.440	39.444	1.00	39.54
C ATOM O		45	OD1	ASN	A	6	69.407	71.747	40.441	1.00	42.37
ATOM		46	ND2	ASN	A	6	68.303	73.414	39.420	1.00	42.40
N ATOM N		<b>47</b> .	N	GLU	A	7	70.263	71.716	34.946	1.00	32.89
ATOM C		48	CA	GLU	A	7	71.158	71.648	33.795	1.00	32.05
ATOM C		49	С	GLU	À	7	70.419	71.313	32.505	1.00	30.13
ATOM O		50	0	GLU	A	7	69.369	70.675	32.528	1.00	30.64
ATOM C		51 '	СВ	GLU	A	7	72.224	70.567	34.012	1.00	34.45
ATOM C		52	CG	GLU	A	7	73.156		35.200	1.00	38.35

ATOM C	53 `	CD	GLU	A	7		74.057	71.981	35.049	1.00	40.20
ATOM O	54	OE1	GLU	Ą	7		74.484	72.278	33.912	1.00	41.55
MOTA O	55	OE2	GLU	A	7		74.351	72.631	36.075	1.00	42.84
ATOM N	56	N	PRO	A	8		70.962	71.745	31.359	1.00	28.48
ATOM C	57	CA	PRO	A	8		70.318	71.446	30.079	1.00	27.48
ATOM C	58	Ċ	PRO	A	8		70.655	69.995	29.755	1.00	26.53
ATOM O	59	0	PRO	A	8		71.59,5	69.448	30.326	1.00	24.18
ATOM C	60	СВ	PRO	A	8		70.992	72.423	29.121	1.00	27.72
ATOM C	61	CG	PRO	A	8		72.380	72.532	29.688	1.00	28.52
ATOM C	62	CĎ	PRO	A	8		72.113	72.649	31.172	1.00	28.72
ATOM N	63	N	CYS	A	9		69.894	69.359	28.869	1.00	26.18
ATOM ,	64	CA	CYS	Α	9		70.202	67.979	28.518	1.00	25.70
ATOM C	65	С	CYS	A	9		71.285	67.935	27.435	1.00	25.71
ATOM O	66 ′	0	CYS	A	9		71.474	68.905	26.685	1.00	24.82 ^
-ATOM C	67	CB	CYS	A	9		68.936	67.239	28.065	1.00	27.09
ATOM S	68	SG	CYS	A	9		68.004	68.021	26.742	1.00	29.97
ATOM N	69	N	HIS	A	10		72.003	66.816	27.370	1.00	24.60
ATOM C	70	CA	HIS	A	10		73.095	66.632	26.414	1.00	24.16
ATOM C	71	С	HIS	Α	10		72.932	65.349	25.612	1.00	24.05
MOTA	72	0	HIS	Ą	10	2	72.269	64.415	26.058	1.00	22.94
ATOM C	73	CB	HIS	A	10	`	74.433	66.580	27.160	1.00	24.38
ATOM C	74	CG	HIS	A	10		74.693	67.779	28.015	1.00	25.68
ATOM N	75	ND1	HIS	Α	10		75.121	68.981	27.498	1.00	26.11
ATOM C	76	CD2	HIS	A	10		74.544	67.973	29.347	1.00	26.09
ATOM C	77	CE1	HIS	A	10		75.225	69.866	28.474	1.00	26.14
ATOM N	78	NEŻ	HIS	A	10	<i>'.</i>	74.879	69.278	29.606	1.00	27.18
ATOM N	79	N	THR	A	.11		73.549	65.311	24.432	1.00	25.34
ATOM C	80	CA	THR	A	11	·	73.494	64.139	23.550	1.00	26.59

ATOM	81	C	THR	A	11		74.857	63.439	23.539	1.00	25.78
C ATOM O	82	0	THR	A	11		75.843	63.990	24.021	1.00	25.20
ATOM C	83	CB	THR	A	11		73.175	64.536	22.095	1.00	28.50
ATOM O	84	OG1	THR	A	11		74.190	65.429	21.620	1.00	31.80
ATOM C	85	CG2	THR	A	11		71.824	65.223	22.000	1.00	31.57
ATOM N	86	N	PHE	A	12		74.909	62.240	22.964	1.00	25.57
MOTA	87	CA	PHE	A	12		76.154	61.469	22.890	1.00	26.57
C ATOM C	88	С	PHE	A	12		77.334	62.201	22.244	1.00	26.75
ATOM O	89	0	PHE	A	12		78.477	62.029	22.666	1.00	26.43
MOTA	90	СВ	PHE	A	12		75.923	60.150	22.139	1.00	26.43
C ATOM	91	CG	PHE	A	12		75.034	59.180	22.869	1.00	27.74
C ATOM C	92	CD1	PHE	A	12	,	75.212	58.940	24.226	1.00	28.25
MOTA	93	CD2	PHE	A	12		74.034	58.490	22.191	1.00	28.95
C ATOM	94	CE1	PHE	A	12		74.405	58.024	24.905	1.00	29.61
C ATOM C	, 95	CE2	PHE	A	12		73.223	57.572	22.858	1.00	29.31
ATOM	96	CZ	PHE	A	12		73.408	57.339	24.215	1.00	29.14
C ATOM	97	N	ASN	A	13		77.071	63.003	21.216	1.00	27.42
N ATOM C	98	CA	ASN	Ą	13	•	78.149	63.726	20.544	1.00	28.91
ATOM C	99	С	ASN	A	13	•	78.892	64.718	21.437	1.00	27.96
MOTA	100	0	ASN	A	13		79.972	65.193	21.076	1.00	28.99
O ATOM C	101	СВ	ASN	A	13		77.621	64.471	19.314	1.00	31.81
ATOM C	102	CG	ASN	Α	13		77.584	63.600	18.079	1.00	34.70
ATOM O	103	OD1	ASN	Α	13		78.485	62.787	17.852	1.00	36.51
ATOM N	104	ND2	2 ASN	Α	13		76.554	63.775	17.261	1.00	37.26
ATOM N	105	N	GLU	Α	14		78.323	65.027	22.596	1.00	26.74
MOTA	106	CA	GLU	Α	14		78.948	65.975	23.517	1.00	26.62
C ATOM C	107	С	GLU	А	14		79.867	65.316	24.541	1.00	26.27
ATOM O	108	0	GLU	A	14		80.414	65.992	25.408	1.00	25.62

ATOM C	109	СВ	GLU .	A	14	77.873	66.763	24.263	1.00 26.66
ATOM C	110	CG	GLU	A	14	76.939	67.529	23.347	1.00 28.65
ATOM C	111	CD	GLU	A	14	75.890	68.293	24.114	1.00 29.22
ATOM O	112	OE1	GLU	A	14	76.260	69.212	24.878	1.00 31.67
MOTA O	113	OE2	GLU	A	14	74.696	67.973	23.957	1.00 29.46
ATOM N	114	N	TÝR	A	15	80.045	64.003	24.439	1.00 25.33
ATOM C	115	CA	TYR	A	15	80.886	63.289	25.391	1.00 25.77
ATOM C	116	С	TYR	A	15	82.069	62.544	24.788	1.00 25.99
ATOM O	117	0	TYR	A	15	82.059	62.152	23.619	1.00 26.38
ATOM ·	118	CB ·	TYR	A	15	80.041	62.279	26.168	1.00 26.71
ATOM C	119	CG	TYR	A	15	79.025	62.889	27.099	1.00 28.01
ATOM C	120	CD1	TYR	A	15	79.377	63.262	28.397	1.00 28.23
ATOM C	121	CD2	TYR	A	15	77.711	63.100	26.683	1.00 29.05
ATOM C	122	CE1	TYR	A	15	78.442	63.828	29.260	1.00 30.46
ATOM C	123	CE2	TYR	A	15	76.771	63.668	27.537	1.00 30.27
ATOM C	124	CZ	TYR	A	15	77.144	64.028	28.820	1.00 30.91
ATOM O	125	ОН	TYR	A	15	76.219	64.604	29.659	1.00 34.07
ATOM N	126	N .	LEU	A	16	83.089	62.350	25.616	1.00 26.06
ATOM C	127	CA	LEU	A	16	84.273	61.593	25.233	1.00 25.76
ATOM C	128	С	LEU	A	16	84.672	60.785	26.457	1.00 24.62
ATOM O	129	0	LEU	A	16	84.331	61.143	27.589	1.00 23.13
ATOM C	130	CB	LEU	A	16	85.427	62.518	24.820	1.00 28.13
ATOM C	131	CG	LEU	A	16 .	85.291	63.282	23.495	1.00 29.82
ATOM C	132	CD1	LEU	A	16	86.523	64.136	23.285	1.00 30.80
ATOM C	133	CD2	LEU	A	16	85.123	62.313	22.332	1.00 30.29
ATOM N	134	N	LEU	A	17	85.374	59:683	26.230	1.00 24.43
ATOM C	135	CA	LEU	A	17	85.841	58.835	27.321	1.00 25.14
ATOM C	136	С	LEU	A	17	87.311	59.147	27.608	1.00 25.20

ATOM O	137	0	LEU	A	17	88.097	59.336	26.682	1.00	25.84
ATOM C	138	СВ	LEU	A	17	85.706	57.359	26.933	1.00	25.29
ATOM C	139	CG	LEU	A	17 .	84.288	56.777	26.938	1.00	25.32
ATOM C	140	CD1	LEU	A	17	84.233	55.534	26.077	1.00	26.22
ATOM C	141	CD2	LEU	A	17	83.876	56.466	28.366	1.00	25.45
ATOM N	142	N	ILE	Α.	18	87.667	59.210	28.889	1.00	25.46
ATOM C	143	CA	ILE	A	18	89.047	59.460	29.294	1.00	25.22
ATOM C	144	С	ILE	A	18	89.608	58.101	29.718	1.00	25.38
MOTA	145	Ο.	ILE	A	18	89.062	57.446	30.598	1.00	25.99
O ATOM C	146	СВ	ILE	A	18	89.112	60.460	30.467	1.00	25.47
ATOM C	147	CG1	ILE	A	18	88.653	61.843	29.979	1.00	25.88
ATOM C	148	CG2	ILE	A	18	90.538	60.531	31.027	1.00	24.00
ATOM C	149	CD1	ILE	A	18	88.620	62.909	31.057	1.00	28.70
ATOM N	150	N	PRO	A .	19	90.701	57.657	29.080	1.00	26.62
ATOM C	151	CA	PRO	A	19	91.306	56.360	29.408	1.00	26.83
ATOM C	152	С	PRO	A	19	91.605	56.116	30.889	1.00	26.38
ATOM O	153	0	PRO	A	19	91.853	57.048	31.656	1.00	26.07
ATOM C	154	CB	PRO	A	19	92.584	56.350	28.564	1.00	27.54
ATOM C	155	CG	PRO	A	19	92.204	57.182	27.371	1.00	28.01
ATOM C	156	CD	PRO	A	19	91.463	58.336	28.018	1.00	27.10
MOTA N	157	N	GLY	A	20,	91.566	54.845	31.271	1.00	25.38
ATOM	158	CA	GLY	A	20	91.877	54.453	32.632	1.00	26.31
C ATOM C	159	С	GLY	A	20	93.077	53.528	32.511	1.00	26.29
MOTA	160	. 0	GLY	A	20	93.662	53.423	31.437	1.00	23.85
ATOM N	, 161	N	LEU	A	21	93.451	52.846	33.585	1.00	26.59
ATOM C	162	CA	LEU	A	21	94.601	51.948	33.506	1.00	27.89
ATOM C	163	С	LEU	Αʻ	21	94.291	50.701	32.690	1.00	28.10
ATOM O	164	0	LEU	A	21	93.361	49.959	33,.002	1.00	28.93

ATOM C	165	СВ	LEU	A	21	95.064	51.536	34.910	1.00	27.80
ATOM C	166	CG	LEU	Α.	21	96.225	50.531	34.941		28.27
ATOM	167	CD1	LEU	A	21 .	97.431	51.084	34.182	1.00	27.34
C ATOM C	168	CD2	LEU	A	21	96.583	50.230	36.390	1.00	29.80
ATOM N	169	N	SER	A	22	95.068	50.483	31.634	1.00	29.02
MOTA	170	CA	SER	A	22	94.900	49.310	30.788	1.00	31.01
C ATOM C	171	. C	SER	Α	22	95.917	48.270	31.238	1.00	32.77
MOTA O	172	. 0	SER	A	22	97.118	48.530	31.234	1.00	31.01
MOTA	173	CB	SER	A	22	95.149	49.663	29.321	1.00	31.45
C ATOM O	174	OG	SER	A	22	94.206	50.608	28.855	1.00	30.59
ATOM N	175	N	THR	A	23	95.435	47.096	31.632	1.00	34.58
ATOM C	. 176	CA	THR	A	23 .	96.322	46.033	32.092	1.00	36.68
MOTA	177	C	THR	A	23	96.716	45.114	30.944	1.00	37.08
C ATOM	178	0	THR	A	23	96.105	45.144	29.875	1.00	37.57
O ATOM C	179	СВ	THR	A	23	95.658	45.207	33.202	1.00	37.62
ATOM O	180	OG1	THR	A	23	94.335	44.851	32.797	1.00	40.83
ATOM C	181	CG2	THR	A	23	95.581	46.011	34.492	1.00	39.51
MOTA N	182	N	VAL	A	24	97.742	44.298	31.163	1.00	37.49
ATOM C	183	CA	VAL	A	24	98.217	43.390	30.128	1.00	38.46
ATOM	184	C	VAL	A	24	97.187	42.348	29.697	1.00	39.49
C ATOM O	185	0	VAL	A	24	97.256	41.832	28.583	1.00	39.42
MOTA	186	CB	VAL	Α	24	99.508	42.660	30.575	1.00	38.44
C ATOM	187	CG1	. VAL	A,	24	100.651	43.662	30.713	1.00	37.27
C ATOM C	188	CG2	VAL	A	24	99.272	41.940	31.894	1.00	38.19
ATOM N	189	N	ASP	Α	25	96.224	42.045	30.562	1.00	41.42
MOTA	190	CA	ASP	Α	25	95.219	41.047	30.210	1.00	44.00
C ATOM	191	С	ASF	A	25	94.070	41.590	29.362	1.00	44.29
C ATOM O	192	0	ASF	A	25	93.220	40.826	28.908	1.00	44.12

ATOM C	193	CB	ASP	A	25	94.653	40.380	31.473	1.00 46.46
ATOM C	194	CG	ASP	A	25	93.826	41.329	32.327	1.00 49.04
ATOM	195	OD1	ASP	A	25	93.177	40.852	33.280	1.00 51.13
O ATOM O	196	OD2	ASP	A	25	93.819	42.545	32.058	1.00 51.46
ATOM N	197	N	CYS	A	26	94.032	42.898	29.132	1.00 44.45
ATOM .	198	CA	CYS	A	26	92.937	43.434	28.333	1.00 44.38
ATOM C	199	С	CYS	Ā	26	93.245	43.623	26.866	1.00 44.52
ATOM O	200	0	CYS	A	26	93.840	44.623	26.465	1.00 44.45
ATOM '	201	CB	CYS	A	26	92.432	44.767	28.879	1.00 43.39
C ATOM S	202	SG	CYS	A	26 .	90.722	45.164	28.351	1.00 43.27
ATOM	203	N	ILE	A	27	92.835	42.646	26.071	1.00 44.85
N ATOM C	204	CA	ILE	A.	27	92.984	42.712	24.631	1.00 45.31
ATOM	205	С	ILE	A	27	91.559	42.482	24.155	1.00 45.02
C ATOM O	206	0	ILE	A	27	90.791	41.782	24.815	1.00 44.66
ATOM C	207	СВ	ILE	A	27	93.924	41.612	24.084	1.00 46.44
MOTA	208	CG1	ILE	A	27	93.461	40.234	24.555	1.00 46.68
C ATOM C	209	CG2	ILE	A	27	95.358	41.893	24.524	1.00 46.86
ATOM C	210	CD1	ILE	A	27	94.354	39.098	24.083	1.00 48.06
ATOM N	211	N	PRO	A	28	91.179	43.089	23.024	1.00 45.29
	2:12	CA	PRO	A	28	89.836	42.959	22.453	1.00 44.96
ATOM C	213	С	PRO	A	28	89.231	41.557	22.486	1.00 44.81
MOTA	214	0	PRO	A	28	88.051	41.393	22.800	1.00 44.44
O ATOM C	215	СВ	PRO	Α.	28	90.027	43.474	21.031	1.00 45.44
ATOM C	216	CG	PRO	A	28	91.024	44.565	,21.223	1.00 45.66
ATOM C	217	CD	PRO	A	28	92.031	43.934	22.166	1.00 45.97
ATOM N	218	N	SER	A	29	90.035	40.549	22.167	1.00 44.03
ATOM C	219	CA	SER	A	29	89.547	39.174	22.134	1.00 43.07
ATOM C	220	C .	SER	A	29	89.168	38.597	23.495	1.00 42.20
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MOTA	221	0	SER	A	29	88.477	37.582	23.567	1.00	42.12
O ATOM C	222	CB	SER	A	29	90.576	38.261	21.455	1.00	43.90
MOTA O	223	OG	SER	A	29	91.766	38.166	22.214	1.00	45.30
MOTA	224	N	ASN	A	30	89.615	39.227	24.575	1.00	40.59
N ATOM . C	225	CA	ASN	A	30	89.271	38.735	25.902	1.00	39.15
ATOM C	226	С	ASN	A	30	88.079	39.489	26.491	1.00	37.08
ATOM	227	0	ASN	A	30	87.606	39.159	27.577	1.00	36.93
O ATOM C	228	CB	ASN	A	30	90.463	38.844	26.858	1.00	41.71
ATOM C	229	CG	ASN	A	30	91.564	37.851	26.538	1.00	44.46
ATOM O	230	OD1	ASN	A	30	91.296	36.703	26.186	1.00	45.63
MOTA	231	ND2	ASN	A	30	92.811	38.283	26.677	1.00	46.20
N ATOM N	232	N	VAL	A	31	87.595	40.497	25.774	1.00	33.45
ATOM	233	CA	VAL	A	31	86.461	41.279	26.252	1.00	31.88
C ATOM	234	С	VAL	A	31	85.150	40.513	26.093	1.00	30.75
C ATOM	235	0	VAL	A	31	84.858	39.981	25.025	1.00	30.55
O	236	СВ	VAL	A	31	86.353	42.628	25.503	1.00	30.76
C ATOM	237	CG1	VAL	A	31	85.074	43.355	25.914	1.00	30.99
C ATOM C	238	CG2	VAL	A	31	87.568	43.491	25.817	1.00	31.39
ATOM N	239	N	ASN	A	32	84.372	40.463	27.168	1.00	30.39
MOTA	240	CA	ASN	A	32	83.085	39.771	27.175	1.00	30.35
C ATOM	241	C -	ASN	A	32	81.968	40.802	27.058	1.00	29.35
C ATOM	242	0	ASN	Α	32	81.837	41.675	27.916	1.00	29.27
O ATOM	243	СВ	ASN	Α	32	82.929	38.965	28.474	1.00	32.17
C ATOM	244	CG	ASN	A	32	81.509	38.449	28.685	1.00	34.34
C ATOM	245	OD1	ASN	Α	32	80.751	38.273	27.736	1.00	34.02
O ATOM	246	ND2	ASN	Α	32	81.153	38.193	29.941	1.00	38.74
N ATOM	247	N	LEU	A	33	81.166	40.705	26.001	1.00	28.15
N ATOM C	248	CA	LEU	A	33	80.077	41.661	25.803	1.00	27.70

ATOM C	249	С	LEU	A	33	78.693	41.128	26.178	1.00	27.94
ATOM O	250	0	LEU	A	33	77.676	41.639	25.711	1.00	27.44
ATOM C	251	CB	LEU	A	33	80.071	42.160	24.351	1.00	27.83
ATOM C	252	CG	LEU	A	33	81.288	42.979	23.906	1.00	28.65
ATOM C	253	CD1	LEU	A	33	81.127	43.403	22.448	1.00	27.96
ATOM C	254	CD2	LEU	Ā	33	81.443	44.202	24.800	1.00	28.65
ATOM N	255	N	SER	A	34	78.646	40.109	27.028	1.00	28.06
ATOM C	256	CA	SER	A	34	77.361	39.559	27.457	1.00	29.26
ATOM C	257	C .	SER	A	34	76.628	40.593	28.310	1.00	28.04
ATOM O	258	0	SER	A	34	77.255	41.406	28.987	1.00	27.93
ATOM C	259	CB .	SER	A	34	77.574	38.283	28.268	1.00	30.15
ATOM O	260	OG	SER	Α	34	78.220	37.308	27.471	1.00	35.29
ATOM N	261	N	THR	A	35	75.301	40.565	28.283	1.00	27.47
ATOM C	262	CA	THR	A	35	74.533	41.528	29.058	1.00	26.66
ATOM C	263	С	THR	A	35	73.113	41.009	29.299	1.00	26.85
ATOM O	264	0	THR	A	35	72.540	40.317	28.455	1.00	27.02
ATOM C	265	CB.	THR	A	35	74.497	42.896	28.320	1.00	27.50
ATOM O	266	OG1	THR	A	35	74.222	43.949	29.252	1.00	27.27
ATOM C	267	CG2	THR	A	35	73.425	42.894	27.234	1.00	26.76
ATOM N	268	N	PRO	A	36	72.529	41.334	30.462	1.00	26.24
ATOM C	269	CA	PRO	`A	36	71.175	40.887	30.795	1.00	26.48
ATOM C	270	Ċ	PRO	A	,36	70.082	41.574	29.979	1.00	26.94
ATOM O	271	0	PRO	A	36	70.166	42.769	29.683	1.00	26.63
ATOM C	272	СВ	PRO	A	36	71.067	41.205	32.282	1.00	25.88
ATOM C	273	CG	PRO ·	A	3.6	71.883	42.446	32.402	1.00	25.82
ATOM C	274	CD	PRO	A	36	73.098	42.144	31.554	1.00	25.46
ATOM N	275	N	LEU	A	37	69.054	40.810	29.627	1.00	26.53
ATOM C	276	CA	LEU	A	37	67.942	41.344	28.857	1.00	26.66

ATOM C	277	С	LEU	A	37	66.705	41.564	29.724	1.00 2	6.63
ATOM O	278	0	LEU	Α.	37	65.960	42.526	29.516	1.00 2	26.36
ATOM C	279	CB	LEU	A	37	67.588	40.396	27.706	1.00 2	27.85
ATOM C	280	CG	LEU	A	37	66.499	40.910	26.759	1.00 2	27.81
ATOM C	281	CD1	LEU	A	37	67.061	42.044	25.911	1.00 2	28.43
ATOM C	282	CD2	LEU	A	37	66.006	39.780	25.869	1.00 2	28.49
MOTA N	283	N	VAL	Α.	38	66.483	40.684	30.699	1.00 2	26.11
ATOM C	284	CA	VAL	A	38	65.305	40.807	31.556	1.00 2	26.61
ATOM C	285	С	VAL	A	38 .	65.651	40.829	33.040	1.00 2	27.13
ATOM	286	0	VAL	A	38	66.667	40.279	33.461	1.00 2	27.11
O ATOM C	287	СВ	VAL	A	38	64.288	39.674	31.264	1.00 2	26.52
ATOM C	288	CG1	VAL	A	38	63.862	39.748	29.803	1.00 2	27.45
MOTA	289	CG2	VAL	A	38	64.902	38.310	31.562	1.00 2	26.40
C ATOM N	290	N	LYS	A	39	64.790	41.468	33.825	1.00 2	27.15
ATOM C	291	CA	LYS	Α	39	65.011	41.625	35.256	1.00, 2	27.73
ATOM C	292	С	LYS	A	39	65.216	40.348	36.058	1.00 2	28.72
ATOM O	293	0	LYS	A	39	64.724	39,274	35.695	1.00 2	28.88
ATOM C	294	CB	LYS	A	39	63.865	42.425	35.885	1.00 2	28.20
ATOM C	295	CG	LYS	A	39	62.508	41.718	35.873	1.00 2	28.09
MOTA	296	CD	LYS	A	39	61.492	42.510	36.690	1.00	29.72
C ATOM C	297	CE	LYS	A	39	60.107	41.877	36.642	1.00	30.35
MOTA	298	NZ	LYS	A	39	59.162	42.618	37.526	1.00	31.05
N ATOM N	299	N	PHE	A	40	65.947	40.502	37.159	1.00	28.59
ATOM C	300	CA	PHE	A	40	66.254	39.424	38.089	1.00	29.38
ATOM .	301	С	PHE	A	40	66.508	40.026	39.469	1.00	30.67
ATOM O	302	0	PHE	A	40	66.605	41.250	39.611	1.00	31.06
ATOM C	303	СВ	PHE	A	40	67.485	38.633	37.627	1.00	29.02
ATOM C	304	CG	PHE	A	40	68.706	39.481	37.379	1.00	28.39

ATOM C	305 _.	CD1	PHE	A	40	68.920	40.074	36.136	1.00 29.01	
ATOM C	306	CD2	PHE	A	40	69.649	39.671	38.381	1.00 28.07	
ATOM	307	CE1	PHE	A	40	70.059	40.843	35.897	1.00 28.63	
C ATOM C	308	CE2	PHE	A	40	70.790	40.435	38.157	1.00 28.51	
ATOM C	309	CZ	PHE	A	40	70.997	41.022	36.912	1.00 28.67	1
ATOM	310	N	GLN	A	41	66.609	39.168	40.482	1.00 30.52	
N ATOM C	311	CA	GLN	A	41	66.843	39.608	41.857	1.00 32.51	-
ATOM C	312	C	GLN	A	41	68.324	39.615	42.199	1.00 31.08	}
MOTA	313	0	GLN	A	41	69.120	38.950	41.544	1.00 32.21	
O ATOM C	314	CB	GLN	A	41	66.131	38.677	42.852	1.00 34.57	7
ATOM C	315	CG	GLN	A	41	64.623	38.683	42.769	1.00 40.18	}
MOTA	316	CD	GLN	A	41	64.029	40.014	43.189	1.00 42.08	}
C ATOM O	317	OE1	GLN	A	41	64.187	40.451	44.333	1.00 45.73	L
ATOM N	318	NE2	GLN	A	41	63.345	40.667	42.263	1.00 44.39	€
MOTA	319	N	LYS	A	42	68.678	40.364	43.238	1.00 30.93	L
N ATOM Č	320	CA	LYS	A	42	70.057	40.444	43.705	1.00 31.44	1
ATOM C	321	С	LYS	A	42	70.606	39.028	43.937	1.00 31.78	3
ATOM	322	0	LYS	·A	42	69.945	38.190	44.556	1.00 30.4	9
O ATOM C	323	СВ	LYS	A	42	70.106	41.241	45.009	1.00 33.1	7
ATOM C	324	CG	LYS	A	42	71.456	41.242	45.701	1.00 35.8	3
ATOM C	325	CD	LYS	A	42	71.399	42.043	46.994	1.00 38.9	2
ATOM	326	CE	LYS	A	42	72.740	42.029	47.706	1.00 40.3	0
C ATOM N	327	NZ	LYS	A	42	72.711	42.865	48.938	1.00 43.5	3
MOTA	328	N	GLY	Α	43	71.805	38.768	43.426	1.00 31.7	6
N ATOM C	329	CA	GLY	A.	43	72.420	37.463	43.593	1.00 31.0	6
ATOM C	330	С	GLY	Α	43	72.125	36.484	42.473	1.00 30.8	1
ATOM O	331	0	GLY	A	43	72.751	35.426	42.384	1.00 30.3	3
ATOM N	332	N	GLN	A	44	71.170	36.822	41.615	1.00 30.1	8

ATOM C	333	CA	GLN	Α	44	70.817	35.946	40.507	1.00	30.45
ATOM .	334	С	GLN	A	44	71.410	36.461	39.203	1.00	31.41
MOTA	335	0	GLN	A	44	72.075	37.494	39.172	1.00	30.58
O ATOM C	336	СВ	GLN	A	44	69.295	35.870	40.345	1.00	31.54
ATOM C	337	CG	GLN	A	44	68.521	35.673	41.637	1.00	32.79
ATOM C	338	CD	GLN	A	44	67.016	35.631	41.407	1.00	34.29
ATOM	339	OE1	GLN	A	44	66.492	36.327	40.537	1.00	32.47
ATOM N	340	NE2	GLN	A	44	66.316	34.827	42.199	1.00	32.10
ATOM	341	N	GLN	A	45	71.161	35.710	38.136	1.00	32.01
N ATOM C	342	CA	GLN	A	45 :	7.1.593	36.058	36.791	1.00	33.43
ATOM C	343	C	GLN	A	45	70.299	36.153	35.992	1.00	32.33
ATOM	344	0	GLN	A	45	69.310	35.516	36.345	1.00	31.57
O ATOM .C	345	СВ	GLN	A	45	72.476	34.957	36.196	1.00	37.06
ATOM C	346	CG	GLN	Ä	45	73.829	34.819	36.864	1.00	42.03
ATOM C	347	CD	GLN	A	45	74.634	36.097	36.781	1,00	44.70
MOTA	348	OE1	GLN	A	45	74.911	36.596	35.689	1.00	47.34
O ATOM N	349	NE2	GLN	A	45	75.010	36.641	37.936	1.00	45.66
MOTA	350	N	SER	A	46	70.299	36.945	34.926	1.00	30.96
N ATOM C	351	CA	SER	A	46	69.103	37.082	34.107	1.00	30.90
ATOM C	352	C .	SER	A	46	68.791	35.762	33.407	1.00	31.56
ATOM O	353	0	SER	A	46	69.700	35.004	33.078	1.00	30.43
MOTA	354	CB	SER	A	46	69.300	38.171	33.053	1.00	29.48
C ATOM O	355	OG	SER	A	46	68.130	38.324	32.276	1.00	28.63
ATOM N	356	N	GLU	A	47	67.507	35.495	33.180	1.,00	32.24
ATOM C	357	CA	GLU	Ä	47	67.097	34.271	32.498	1.00	33.72
ATOM C	358	С	GLU	A	47	67.495	34.336	31.033	1.00	32.95
ATOM	359	0 -	GLU	A	47	67.601	33.311	30.363	1.00	32.68
ATOM C	360	СВ	GLU	A	47	65.587	34.078	32.614	1.00	35.36

ATOM C	361	CG	GLU	A	47	65.118	33.791	34.027	1.00	39.32
ATOM C	362	CD	GLU	A	47	63.613	33.865	34.159	1.00	41.79
MOTA O	363	OE1	GLU	A	47	62.918	33.052	33.513	1.00	44.11
ATOM O	364	OE2	GLU	A	47	63.124	34.743	34.904	1.00	43.26
ATOM N	365	N	ILE	A	48	67.701	35.551	30.531	1.00	31.57
ATOM C	366	CA	ILE	A	48	68.114	35.736	29.143	1.00	30.16
ATOM C	367	С	ILE	A	48	69.271	36.727	29.080	1.00	29.80
ATOM O	368	0	ILE	A	48	69.148	37.869	29.521	1.00	29.23
ATOM C	369	CB	ILE	A	48 _	66.962	36.280	28.258	1.00	31.15
ATOM C	370	CG1	ILE	A	48	65.780	35.308	28.267	1.00	31.70
ATOM C	371	CG2	ILE	A	48	67.461	36.479	26.835	1.00	30.35
ATOM C	372	CD1	ILE	A.	48	64.578	35.800	27.487	1.00	33.88
ATOM N	373	N	ASN	A	49	70.396	36.280	28.536	1.00	28.20
ATOM C	374	CA	ASN	A	49	71.567	37.129	28.403	1.00	28.79
ATOM C	375	С	ASN	A	49	71.982	37.194	26.947	1.00	28.45
MOTA	376	0	ASN	A	49	72.204	36.160	26.309	1.00	28.24
O ATOM C	377	CB	ASN	A	49	72.728	36.579	29.238	1.00	29.15
ATOM .	378	CG	ASN	A	49	72.459	36.656	30.726	1.00	30.85
ATOM O	379	OD1	ASN	A	49	72.610	37.712	31.343	1.00	29.61
ATOM N	380	ND2	ASN	A	49	72.041	35.538	31.310	1.00	30.46
ATOM N	381	N	LEU	A	50	72.061	38.407	26.412	1.00	27.38
ATOM C	382	CA	LEU	A	50	72.488	38.585	25.030	1.00	27.41
ATOM C	383	С	LEU	A	50	73.990	38.324	25.035	1.00	27.31
ATOM O	384	0	LEU	·A	50	74.635	38.498	26.069	1.00	26.24
ATOM C	385	CB	LEU	A	50	72.233	40.026	24.573	1.00	27.05
ATOM C	386	CG	LEU	A	50	70.818	40.596	24.686	1.00	28.18
ATOM C	387	CD1	LEU	A	50	70.838	42.092	24.356	1.00	28.26
ATOM C	388	CD2	LEU	A	50	69.887	39.849	23.745	1.00	29.22

ATOM N	389	N	LYS	A	51	74.542	37.898	23.901	1.00 28.23
ATOM C	390	CA	LYS	A	51	75.978	37.666	23.804	1.00 28.76
ATOM C	391	С	LYS	A	51	76.661	38.946	23.313	1.00 28.00
ATOM O	392	0	LYS	A	51	77.867	39.118	23.478	1.00 27.68
ATOM C	393	CB	LYS	A	51	76.275	36.463	22.897	1.00 31.27
ATOM C	394	CG	LYS	A	51	75.819	35.155	23.546	1.00 32.77
ATOM C	395	CD	LYS	A	51	76.238	33.915	22.771	1.00 35.29
ATOM C	396	CE	LYS	A	51	75.732 ·	32.661	23.486	1.00 36.18
ATOM N	397	NZ	LYS	A	51	76.082	31.402	22.757	1.00 38.13
ATOM N	398	N	ILE	A	52	75.877	39.834	22.700	1.00 26.71
ATOM C	399	CA .	ILE	A .	<b>52</b>	76.359	41.150	22.277	1.00 26.00
ATOM C	400	С	ILE	A	52	75.227	42.109	22.668	1.00 26.56
MOTA	401	0	ILE	A	52	74.049	41.764	22.566	1.00 26.00
O ATOM C	402	CB	ILE	A	52	76.689	41.247	20.756	1.00 26.91
ATOM C	403	CG1	ILE	A	52	75.458	40.947	19.899	1.00 27.54
ATOM C	404	CG2	ILE	A	52	77.856	40.303	20.421	1.00 27.36
ATOM	405	CD1	ILE	A	52	75.675	41.287	18.423	1.00 27.06
MOTA N	406	N	PRO	A	53	75.570	43.322	23.124	1.00 25.59
	407	CA	PRO	A	53	74.590	44.326	23.556	1.00 26.47
ATOM C	408	С	PRO	A	53	73.782	45.080	22.501	1.00 27.16
ATOM O	409	0	PRO	A	53	73.395	46.228	22.730	1.00 26.78
ATOM C	410	CB	PRO	A	53	75.439	45.269	24.400	1.00 25.56
ATOM C	411	CG	PRO	A	53	76.720	45.315	23.605	1.00 25.49
ATOM C	412	CD	PRO	A	53	76.945	43.853	23.222	1.00 25.76
ATOM N	413	N	LEU	A	54	73.502	44.443	21.368	1.00 26.87
MOTA	414	CA	LEU	Α	54	72.745	45.106	20.314	1.00 27.02
C ATOM C	415	С	LEU	Α	54	71.426	44.404	19.979	1.00 26.78
ATOM O	416	0	LEU	Α	54	71.376	43.177	19.861	1.00 27.27

ATOM C	417	СВ	LEU	A	54	73.588	45.201	19.038	1.00	26.49
ATOM C	418	CG	LEU	A	54	75.010	45.771	19.104	1.00	26.90
ATOM C	419	CD1	LEU	A	54	75.588	45.807	17.692	1.00	28.33
ATOM C	420	CD2	LEU	A	54	75.000	47.168	19.716	1.00	26.89
ATOM N	421	N	VAL	Α	55	70.359	45.186	19.847	1.00	26.28
ATOM C	422	CA	VAL	A	55	69.061	44.641	19.461	1.00	26.52
ATOM C	423	С	VAL	A	55	68.516	45.542	18.349	1.00	26.85
ATOM . O	424	0	VAL	A	55	68.753	46.751	18.353	1.00	27.05
ATOM C	425	СВ	VAL	A	55	68.066	44.574	20.655	1.00	26.19
ATOM C	426	CG1	VAL	A	55	68.718	43.837	21.823	1.00	25.91
ATOM C	427	CG2	VAL	Α	55	67.614	45.963	21.064	1.00	26.54
ATOM N	428	N	SER	Α	56	67.812	44.958	17.381	1.00	26.45
ATOM C	429	CA	SER	A	56	67.281	45.750	16.279	1.00	26.33
ATOM C	430	С	SER	A	56	65.909	46.329	16.613	1.00	26.47
ATOM O	431	0	SER	A	56	65.091	45.694	17.286	1.00	26.78
ATOM C	432	CB	SER	A	56	67.239	44.916	14.985	1.00	27.61
ATOM O	433	OG	SER	A	56	66.504	43.720	15.149	1.00	27.08
ATOM N	434	N	ALA	A	57	65.687	47.556	16.152	1.00	26.29
ATOM C	435	CA	ALA	A	57	64.462	48.307	16.400	1.00	26.64
ATOM C	436	С -	ALA	A	57	63.167	47.618	15.963	1.00	27.43
ATOM O	437	0	ALA	A	57	63.161	46.798	15.045	1.00	27.98
ATOM C	438	СВ	ALA	A	57	64.572	49.672	15.739	1.00	25.98
ATOM N	439	N	ILE	A	58	62.076	47.968	16.638	1.00	27.92
ATOM C	440	CA	ILE	A	58	60.753	47.413	16.354	1.00	28.86
ATOM C	441	С	ILE	A	58	60.196	48.224	15.191	1.00	29.07
ATOM O	442	0	ILE	A	58	59.308	49.064	15.371	1.00	29.42
ATOM C	443	СВ	ILE	A	58	59.823	47.572	17.576	1.00	28.92
ATOM C	444	CG1	ILE	A	58	60.574	47.170	18.852	1.00	28.75

ATOM	445	CG2	ILE	A	58		58.578	46.718	17.397	1.00	27.62
C ATOM C	446	CD1	ILE	A	58		59.752	47.286	20.126	1.00	29.63
ATOM	447	N	MET	A	59		60.731	47.969	14.003	1.00	29.21
N ATOM	448	CA	MET	A	59		60.344	48.714	12.811	1.00	29.85
C ATOM C	449	С	MET	A	59		60.187	47.851	11.565	1.00	30.08
ATOM	450	0	MET	A	59		60.970	46.929	11.330	1.00	29.39
O ATOM	451	СВ	MET	A	59		61.395	49.793	12.537	1.00	29.69
C ATOM C	452	CG	MET	A	59		61.639	50.736	13.710	1.00	29.89
MOTA	453	SD	MET	A	59		63.017	51.863	13.414	1.00	30.04
S ATOM	454	CE	MET	A	59		62.383	52, 830	12.049	1.00	28.55
C ATOM N	455	N .	GLN	A	60		59.182	48.181	10.756	1.00	30.89
ATOM	456	CA	GLN	A	60		58.906	47.452	9.520	1.00	31.91
C ATOM	457	С	GLN	A	60		60.127	47.431	8.606	1.00	32.39
C ATOM	458	0	GLN	A	60		60.374	46.447	7.916	1.00	32.51
O ATOM	459	СВ	GLN	A	60		57.759	48.110	8.741	1.00	32.69
ATOM	460	CG	GLN	A	60		56.508	48.441	9.532	1.00	33.24
C ATOM C	461	CD	GLN	A	60		55.445	49.085	8.656	1.00	35.53
ATOM O	462	OE1	GLN	A	60		55.761	49.829	7.723	1.00	35.53
ATOM N	463	NE2	GLN	A	60		54.178	48.813	8.957	1.00	35.36
MOTA	464	N	SER	A	61	· _	60.879	48.528	8.590	1.00	-32.34
N ATOM C	465	CA	SER	A	61		62.051	48.629	7.727	1.00	32.96
ATOM	466	С	SER	A	61		63.333	48.085	8.344	1.00	32.88
C ATOM O	467	0	SER	A	61		64.415	48.273	7.790	1.00	34.10
ATOM C	468	СВ	SER	A	61		62.273	50.089	7.312	1.00	33.69
ATOM O	469	OG	SER	A	61		62.544	50.910	8.437	1.00	35.94
ATOM	470	N	VAL	A	62		63.218	47.394	9.472	1.00	32.07
N ATOM C	471	CA	VAL	A	62		64.404	46.867	10.130	1.00	31.11
ATOM C	472	С	VAL	A	62		64.348	45.411	10.572	1.00	31.10

ATOM O	473	ο .	VAL	A	62	65.145	44.590	10.126	1.00	31.19
ATOM.	474	CB	VAL	A	62	64.764	47.713	11.383	1.00	31.46
ATOM	475	CG1	VAL	A	62	65.992	47.128	12.070	1.00	30.28
C ATOM C	476	CG2	VAL	A	62	65.018	49.160	10.988	1.00	30.77
ATOM N	477	N	SER	A	63	63.399	45.091	11.444	1.00	31.39
ATOM C	478	CA	SER	A	63	63.312	43.752	12.000	1.00	31.57
ATOM C	479	С	SER	A	63	62.341	42.743	11.393	1.00	32.24
ATOM O	480	0	SER	A	63	61.242	42.535	11.907	1.00	31.09
ATOM	481	CB	SER	A	63	63.064	43.863	13.508	1.00	31.83
C ATOM O	482	OG	SER	A	63	64.118	44.590	14.129	1,.00	31.09
ATOM	483	N	GLY	A	64	62.778	42.112	10.307	1.00	32.50
N ATOM C	484	CA	GLY	A	64	61.986	41.087	9.651	1.00	34.07
ATOM	485	C	GLY	A	64	62.598	39.756	10.051	1.00	35.58
C ATOM O	486	0	GLY	Α	64	63.493	39.729	10.903	1.00	33.57
ATOM	487	N	GLU	A	65	62.155	38.652	9.450	1.00	36.69
N ATOM	488	CA	GLU	Α	65	62.704	37.350	9.821	1.00	38.49
C ATOM C	489	С	GLU	A	65	64.187	37.205	9.494	1.00	38.04
ATOM O	490	0	GLU	A	65	64.942	36.652	10.292	1.00	37.92
ATOM C	491	СВ	GLU	A	65	61.913	36.202	9.171	1.00	41.36
ATOM	492	CG	GLU	A	65	61.881	36.201 -	7.652	1.00	46.27
ATOM C	493	CD	GLU	A	65	60.758	37.049	7.076,	1.00	49.42
MOTA	494	OE1	GLU	A	65	60.603	37.055	5.835	1.00	51.56
O ATOM O	495	OE2	GLU	A	65	60.028	37.706	7.852	1.00	51.36
ATOM N	496	N	LYS	A	66	64.606	3.7.700	8.333	1.00	37.76
ATOM	497	CA	LYS	A	66	66.006	37.612	7.934	1.00	38.96
C ATOM	498	С	LYS	A	66	66.909	38.345	8.924	1.00	37.51
C ATOM	499	0	LYS	A	66	67.975	37.848	9.290	1.00	36.95
O ATOM C	500	CB	LYS	A	66	66.208	38.193	6.531	1.00	40.79

ATOM C	501	CG	LYS	A	66	65.594 ·	37.358	5.415	1.00	45.49
ATOM C	502	CD	LYS	A	66	65.912	37.944	4.042	1.00	48.08
ATOM C	503	CE	LYS	A	66	65.320	37.094	2.925	1.00	49.82
ATOM N	504	NZ	LYS	A	66	65.647	37.631	1.571	1.00	51.36
ATOM N	505	N	MET	A	67	66.480	39.527	9.351	1.00	35.99
ATOM C	506	CA	MET	A	67	67.254	40.314	10.304	1.00	34.82
ATOM C	507	С	MET	A	67	67.378	39.563	11.624	1.00	34.24
ATOM O	508	0	MET	A	67	68.468	39.447	12.182	1.00	33.61
ATOM C	509	CB	MET	A	67	66.579	41.666	10.545	1.00	34.96
ATOM C	510	CG	MET	A	67	67.298	42.561	11.546	1.00	34.38
ATOM S	511	SD	MET	A	67	68.955	43.020	11.010	1.00	35.01
ATOM C	512	CE	MET	A	67	68.573	44.146	9.657	1.00	33.42
ATOM N	513	N	ALA	A	68	66.252	39.046	12.110	1.00	33.39
ATOM C	514	CA	ALA	A	68	66.215	38.315	13.369	1.00	33.20
ATOM C	515	С	ALA	A	68	67.165	37.123	13.387	1.00	33.51
MOTA	516	0	ALA	A	68	67.798	36.841	14.403	1.00	33.13
O ATOM C	517	СВ	ALA	A	68	64.787	37.854	13.661	1.00	33.11
ATOM N	518	N	ILE	A	69	67.262	36.419	12.265	1.00	33.68
ATOM C	519	CA	ILE	A	69	68.147	35.265	12.182	1.00	33.04
ATOM C	520	С	ILE	A	69	69.603	35.712	12.131	1.00	32.05
ATOM O	521	0	ILE	Α.	69	70.452	35.174	12.841	1.00	33.24
ATOM C	522	CB	ILE	A	69	67.827	34.409	10.933	1.00	34.02
ATOM C	523	CG1	ILE	A	69	66.463	33.736	11.104	1.00	34.34
ATOM C	524	CG2	ILE	A	69	68.911	33.365	10.719	1.00	33.54
ATOM C	525	CD1	ILE	A	69	65.913	33.127	9.819	1.00	37.29
ATOM N	526	N	ALA	A	70	69.884	36.709	11.300	1.00	31.48
ATOM C	527	CA	ALA	A	70	71.236	37.225	11.149	1.00	30.65
ATOM C	528	С	ALA	A	70	71.799	37.799	12.445	1.00	30.57

ATOM O	529	0	ALA	A	70	72.969	37.593	12.763	1.00	29.93
ATOM C	530	СВ	ALA	A	70	71.264	38.284	10.063	1.00	30.23
ATOM	531	N	LEU	A	71	70.967	38.523	13.188	1.00	29.53
N ATOM C	532	CA	LEU	A	71	71.409	39.129	14.438	1.00	29.98
ATOM C	533	С	LEU	A	71	71.553	38.098	15.552	1.00	30.25
ATOM O	534	0	LEU	A	71	72.517	38.141	16.314	1.00	30.96
ATOM C	535	CB	LEU	A	71	70.442	40.242	14.859	1.00	28.55
ATOM C	536	CG	LEU	A	71	70.809	41.061	16.103	1.00	28.68
ATOM C	537	CD1	LEU	A	71	72.271	41.482	16.041	1.00	27.67
ATOM C	538	CD2	LEU	A	71	69.898	42.287	16.192	1.00	28.74
ATOM	539	N .	ALA	A	72	70.607	37.166	15.645	1.00	31.21
N ATOM C	540	CA	ALA	Α	72	70.683	36.131	16.672	1.00	31.98
ATOM	541	C	ALA	A	72	71.953	35.308	16.468	1.00	32.78
C ATOM O	542	0	ALA	Α	72	72.569	34.847	17.434	1.00	31.74
ATOM	543	CB	ALA	A	72	69.452	35.222	16.608	1.00	31.69
C ATOM	544	N	ARG	A	73	72.335	35.121	15.206	1.00	33.82
ATOM C	545	CA	ARG	A	73	73.533	34.354	14.876	1.00	35.76
ATOM C	546	С	ARG	A	73	74.786	35.010	15'.435	1.00	35.30
ATOM	547	0	ARG	A	73	75.760	34.328	15.745	1.00	34.89
O ATOM C	548	СВ	ARG	Α	73	73.680	34.200	13.358	1.00	37.37
ATOM C	549	CG __	ARG	A	73	72.809	33.109	12.747	1.00	39.96
ATOM	550	CD	ARG	A	73	72.927	33.093	11.228	1.00	42.81
C ATOM N	551	NE	ARG	A	73	72.204	31.970	10.636	1.00	45.35
ATOM	552	CZ	ARG	A	73	71.945	31.844	9.337	1.00	47.16
C ATOM N	553	NH1	ARG	A	73	72.344	32.773	8.479	1.00	47.06
ATOM N	554	NH2	ARG	A	73	71.289	30.778	8.894	1.00	48.38
ATOM ·	555	N	GLU	A	74	74.755	36.335	15.565	1.00	35.55
ATOM C	556	CA	GLU	A	74	75.899	37.069	16.088	1.00	34.99

ATOM C	557	С	GLU	A	74	75.796	37.327	17.591	1.00	33.84
ATOM O	558	0	GLU	A	74	76.693	37.923	18.181	1.00	33.27
ATOM C	559	CB	GLU	A	74	76.065	38.396	15.342	1.00	37.11
ATOM C	560	ĊG	GLU	A	74	76.218	38.254	13.826	1.00	39.97
ATOM C	561	CD	GLU	A	74	77.309	37.270	13.418	1.00	43.26
MOTA O	562	OE1	GĻŪ	A	74	78.448	37.383	13.924	1.00	44.46
ATOM O	563	OE2	GLU	A	74	77.027	36.384	12.580	1.00	44.73
ATOM N	564	N	GLY	A	75	74.702	36.893	18.209	1.00	32.10
ATOM	565	CA	GLY	A	75	74.562	37.081	19.645	1.00	31.13
C ATOM C	566	С	GLY	A	75	73.553	38.107	20.123	1.00	30.09
ATOM O	567	0	GLY	A	75	73.352	38.256	21.330	1.00	29.67
ATOM	568	N	GLY	A	76	72.926	38.815	19.190	1.00	28.66
N ATOM C	569	CA	GLY	A	76	71.937	39.814	19.559	1.00	28.32
ATOM C	570	С	GLY	A	76	70.526	39.294	19.342	1.00	28.09
ATOM	571	0	GLY	A	76	70.325	38.101	19.089	1.00	27.76
O ATOM N	572	N	ILE	A	77	69.541	40.181	19.436	1.00	27.98
ATOM C	573	CA	ILE	A	77	68.157	39.774	19.239	1.00	27.37
ATOM C	574	С	ILE	A	77	67.363	40.857	18.497	1.00	28.41
ATOM O	575	0	ILE	A	77	67.632	42.053	18.638	1.00	26.87
ATOM C	576	СВ	ILE	A	77	67.491	39.456	20.603	1.00	27.78
ATOM C	577	CG1	ILE	A	77 .	66.246	38.592	20.392	1.00	27.09
ATOM	578	CG2	ILE	A	77	67.128	40.757	21.337	1.00	26.59
C ATOM C	579	CD1	ILE	A	77	65.560	38.187	21.679	1.00	25.93
ATOM N	580	N	SER	A	78	66.404	40.430	17.682	1.00	28.44
ATOM C	581	CA	SER	A	78	65.570	41.364	16.936	1.00	28.97
ATOM C	582	C ·	SER	A	78	64.167	41.354	17.512	1.00	28.83
ATOM O	583	0	SER	A	78	63.714	40.342	18.041	1.00	28.85
ATOM C	584	СВ	SER	A	78	65.487	40.971	15.457	1.00	27.56

ATOM O	585	OG	SER	A	78	66.716	41.168	14.790	1.00	28.48
ATOM N	586	N	PHE	A	79	63.487	42.490	17.418	1.00	29.16
ATOM C	587	CA	PHE	A	79	62.117	42.591	17.893	1.00	29.89
ATOM C	588	C .	PHE	A	79	61.237	42.769	16.668	1.00	30.19
ATOM O	589	0	PHE	A	79	61.060	43.879	16.176	1.00	30.27
ATOM C	590	CB	PHE	A	79	61.941	43.779	18.847	1.00	29.28
ATOM C	591	CG	PHE	A	79	62.503	43.536	20.216	1.00	29.03
ATOM C	592	CD1	PHE	A	79	63.855	43.737	20.477	1.00	30.34
ATOM C	-593	CD2	PHE	A	79	61.687	43.061	21.237	1.00	29.64
ATOM C	594	CE1	PHE	A	79	64.387	43.467	21.741	1.00	30.52
ATOM C	595	CE2	PHE	A	79	62.207	42.786	22.502	1.00	30.51
ATOM C	596	CZ	PHE	A	79	63.561	42.990	22.753	1.00	29.61
ATOM N	597	N	ILE	A	80	60.708	41.656	16.170	1.00	31.21
ATOM C	598	ĊĀ	ILE	A	80	59.844	41.659	14.993	1.00	30.53
ATOM C	599	С	ILE	<b>A</b> .	80	58.766	42.728	15.137	1.00	30.49
ATOM O	600	0	ILE	A	80	58.047	42.761	16.143	1.00	30.23
ATOM C	601	СВ	ILE	A	80	59.172	40.282	14.809	1.00	30.87
ATOM C	602	CG1	ILE	A	80	60.240	39.187	14.721	1.00	30.68
ATOM C	603	CG2	ILE	A	80	58.303	40.288	13.561	1.00	31.61
ATOM C	604	CD1	ILE	A	80	61.174	39.319	13.536	1.00	30,.88
ATOM N	605	N	PHE	A	81	58.640	43.591	14.131	1.00	30.29
ATOM C	606	CA	PHE	A	81	57.660	44.666	14.195	1.00	
ATOM C	607	c.	PHE	A	81	56.216	44.205	14.385	1.00	32.15
ATOM O	608	0	PHE	A	81	55.799	43.178	13.851	1.00	32.55
ATOM C	609	CB	PHE	A	81	57.775	45.593	12.967	1.00	31.76
ATOM C	610	CG	PHE	A	81	57.565	44.914	11.638	1.00	31.76
ATOM C	611	CD1	PHE	A	81	58.575	44.152	11.055	1.00	31.23
ATOM C	612	CD2	PHE	A	81	56.370	45.084	10.942	1.00	31.53

ATOM C	613	CE1	PHE	A	81	58.401	43.574	9.793	1.00 31.24
ATOM C	614	CE2	PHE	A	81	56.184	44.510	9.681	1.00 31.41
ATOM C	615	CZ	PHE	A	81	57.202	43.755	9.106	1.00 32.04
ATOM N	616	N	GLY	A	82	55.467	44.976	15.168	1.00 32.45
ATOM C	617	CA	GLY ·	A	82	54.080	44.652	15.443	1.00 33.29
ATOM C	618	С	GLY	A	82	53.117	45.479	14.616	1.00 34.37
ATOM O	619	0	GLY	A	82	51.899	45.351	14.761	1.00 34.23
ATOM N	620	N	SER	A	83	53.661	46.335	13.756	1.00 34.06
ATOM C	621	CA	SER	A	83	52.844	47.173	12.886	1.00 34.88
ATOM C	622	С	SER	A	83	52.470	46.370	11.645	1.00 35.53
ATOM O	623	0	SER	A	83	52.775	46.745	10.513	1.00 34.34
ATOM C	624	СВ	SER	A	83	53.607	48.440	12.491	1.00 34.13
ATOM O	625	OG	SER	A	83	54.875	48.115	11.961	1.00 35.16
ATOM N	626 '	N	GLN	A	84	51.823	45.238	11.893	1.00 36.05
ATOM C	627	CĀ	GLN	A	84	51.359	44.337	10.851	1.00 36.48
ATOM C	628	С	GLN	A	84	50.308	43.459	11.520	1.00 36.44
ATOM O	629	0	GLN	A	84	50.125	43.532	12.737	1.00 35.78
ATOM C	630	СВ	GLN	A	84	52.515	43.488	10.317	1.00 36.59
ATOM C	631	CG	GLN	A	84	53.156	42.571	11.342	1.00 37.16
	632	CD.	GLN	A,	84	54.277	41.745	10.747	1.00 37.80
	633	OE1	GLN	A	84	54.114	41.137	9.689	1.00 38.49
ATOM N	634	NE2	GLN	A	84	55.422	41.710	11.428	1.00 36.72
ATOM N	635	N	SER	A	85	49.617	42.634	10.742	1.00 37.40
ATOM C	636	CA	SER	A	85	48.582	41.775	11.307	1.00 37.95
ATOM C	637	С	SER	A	85	49.166	40.812	12.333	1.00 38.81
ATOM O	638	0	SER	A	85	50.351	40.479	12.283	1.00 39.00
ATOM C	639	CB	SER	A	85	47.886	40.974	10.205	1.00 37.33
ATOM O	640	OG	SER	A	85	48.700	39.902	9.768	1.00 38.10

ATOM N	641	N	ILE	A	86	48.325	40.372	13.262	1.00	38.89
ATOM C	642	CA	ILE	A	86	48.742	39.439	14.301	.1.00	40.23
ATOM C	643	С	ILE	A	86	49.236	38.140	13.665	1.00	41.35
ATOM O	644	0	ILE	A	86	50.240	37.569	14.090	1.00	41.06
ATOM C	645	CB	ILE	A	86	47.569	39.127	<b>1</b> 5.261	1.00	40.08
ATOM C	646	CG1	ILE	A	86	47.192	40.391	16.041	1.00	40.14
ATOM C	647	CG2	ILE	A	86	47.945	37.992	16.203	1.00	39.43
ATOM C	648	CD1	ILE	A	86	46.003	40.226	16.973	1.00	39.32
ATOM N	649	N	GLU	A	87	48.525	37.687	12.638	1.00	41.92
ATOM C	650	ĊA	GLU	A	87	48.877	36.460	11.932	1.00	42.93
ATOM C	651	С	GLU	A	87	50.228	36.595	11.230	1.00	41.66
ATOM	652	0	GLU	A	87	51.057	35.687	11.272	1.00	41.43
O ATOM C	653	CB	GLU	A	87	47.800	36.122	10.893	1.00	45.26
ATOM C	654	CG	GLU	A	87	46.395	35.876	11.460	1.00	48.53
ATOM C	655	CD	GLU	A·	87	45.798	37.088	12.173	1.00	50.40
ATOM	656	OE1	GLU	A	87	45.867	38.211	11.625	1.00	50.61
O ATOM O	657	OE2	GLU	A	87	45.243	36.910	13.282	1.00	52.40
ATOM N	658	N	SER	A	88	50.439	37.736	10.585	1.00	40.93
ATOM C	659	CA	SER	A	88	51.677	37.993	9.857	1.00	41.02
ATOM C	660	С	SER	A	88	52.898	38.079	10.777	1.00	39.71
ATOM O	661	0	SER	A	88	53.979	37.595	10.438	1.00	39.05
ATOM C	662	СВ	SER	A	88	51.540	39.292	9.058	1.00	41.43
ATOM O	663	OG	SER	A	88	52.675	39.507	8.242	1.00	44.62
ATOM N	664	N	GLN	A	89	52.726	38.701	11.938	1.00	38.95
ATOM C	665	CA	GLN	A	89	53.827	38.837	12.886	1.00	38.02
ATOM C	666	С	GLN	A	89	54.165	37.484	13.506	1.00	38.23
ATOM O	667	0	GLN	A	89	55.333	37.121	13.625	1.00	38.13
ATOM C	668	СВ	GLN	A	89	53.465	39.847	13.984	1.00	36.71

ATOM	669	CG	GLN	A	89	54.536	40.002	15.067	1.00	34.83
C ATOM	670	CD	GLN	A	89	54.169	41.044	16.110	1.00	33.42
C				_	0.					
ATOM O	671	OE1	GLN	A	89	52.998	41.217	16.443	1.00	32.85
ATOM N	672	NE2	GLN	A	89	55.175	41.732	16.644	1.00	31.51
ATOM N	673	N	ALA	A	90	53.137	36.734	13.890	1.00	38.39
ATOM C	674	CA	ALA	A	90	53.343	35.419	14.487	1.00	38.40
ATOM C	675	С	ALA	A	90	54.050	34.494	13.500	1.00	38.83
ATOM O	.676	0	ALA	A	90	54.847	33.639	13.894	1.00	38.82
ATOM C	677	CB	ALA	A	90	52.006	34.822	14.908	1.00	38.88
ATOM N	678	N	ALA	A	91	53.762	34.670	12.215	1.00	39.13
ATOM C	679	CA	ALA	A	91	54.383	33.849	11.186	1.00	39.02
ATOM C	680	С	ALA	A	91	55.893	34.091	11.157	1.00	39.29
ATOM O	681	0	ALA	A	91	56.673	33.150	11.035	1.00	38.36
ATOM C	682	СВ	ALA	A	91	53.767	34.157	9.820	1.00	39.60
ATOM N	683	N	MET	A	92	56.306	35.351	11.272	1.00	38.81
ATOM C	684	CA	MET	A	92	57.733	35.670	11.263	1.00	38.78
ATOM C	685	С	MET	A	92	58.426	35.071	12.480	1.00	37.97
ATOM O	686	0	MET	A	92	59.518	34.516	12.369	1.00	38.17
ATOM C	687	СВ	MET	A	92	57.959	37.184	11.251	1.00	38.46
ATOM C	688	CG	MET	A	92	57.461	37.876	10.009	1.00	39.51
ATOM S	689	SD	MET	A	92	57.978	39.598	9.950	1.00	38.93
ATOM C	690	CE	MET	A	92	57.344	40.065	8.337	1.00	39.38
ATOM N	691	N	VAL	A	93	57.789	35.193	13.641	1.00	37.66
ATOM C	692	CA	VAL	A	93	58.348	34.649	14.872	1.00	37.49
ATOM C	693	С	VAL	A	93	58.501	33.136	14.725	1.00	38.78
ATOM O	694	0	VAL	A	93	59.547	32.572	15.042	1.00	37.88
ATOM C	695	СВ	VAL	A	93	57.434	34.951	16.082	1.00	37.04
ATOM C	696	CG1	VAL	A	93	57.888	34.152	17.294	1.00	36.02

ATOM C	697	CG2	VAL	A	93	57.460	36.443	16.394	1.00	36.04
ATOM N	698	N	HIS	A	94	57.451	32.486	14.231	1.00	39.37
ATOM C	699	CA	HIS	A	94	57.474	31.039	14.040	1.00	39.99
ATOM C	700	С	HIS	A	94	58.616	30.632	13.110	1.00	39.10
ATOM O	701	0	HIS	A	94	59.331	29.663	13.378	1.00	39.42
ATOM C	702	СВ	HIS	A	94	56,144	30.560	13.449	1.00	41.81
ATOM C	703	CG	HIS	A	94	56.048	29.072	13.312	1.00	43.35
ATOM N	704	ND1	HIS	A	94	55.746	28.244	14.372	1.00	44.55
ATOM C	705	CD2	HIS	A	9'4	56.249	28.261	12.247	1.00	44.14
ATOM C	706	CE1	HIS	A	94	55.765	26.987	13.966	1.00	44.38
ATOM N	707	NE2	HIS	A	94	56.069	26.970	12.681	1.00	44.90
ATOM N	708	N	ALA	A	95	58.784	31.377	12.022	1.00	38.67
ATOM C	709	CA	ALA	A	95	59.828	31.093	11.043	1.00	38.33
ATOM C	710	С	ALA	A	95	61.224	31.175	11.648	1.00	38.74
ATOM O	711	0	ALA	A	95	62.107	30.393	11.299	1.00	37.70
ATOM C	712	CB	ALA	A	95	59.717	32.055.	9.866	1.00	38.60
ATOM N	713	N	VAL	A	96	61.429	32.126	12.554	1.00	38.74
ATOM C	714	CA	VAL	A	96	62.732	32.279	13.186	1.00	38.66
ATOM C	715	С	VAL	A	96	62.972	31.145	14.179	1.00	38.92
ATOM O	716	0	VAL	A	96	64.054	30.558	14.212	1.00	39.96
ATOM C	717	CB	VAL	À	96	62.843	33.640	13.920	1.00	38.15
	718	CG1	VAL	A	96	64.174	33.738	14.642	1.00	37.72
	719	CG2	VAL	A	96	62.709	34.776	12.919	1.00	38.27
ATOM N	720	N	LYS	A	97	61.958	30.828	14.976	1.00	39.73
ATOM C	721	CA	LYS	A	97	62.081	29.767	15.969	1.00	40.96
ATOM C	722	С	LYS	A	97	62.273	28.383	15.351	1.00	42.44
ATOM O	723	0	LYS	A	97	62.860	27.502	15.977	1.00	42.21
ATOM C	724	СВ	LYS	A	97	60.856	29.750	16.892	1.00	40.24

ATOM C	725	CG	LYS	A	. 97	60.659	31.021	17716	1.00	39.72
ATOM C	726	CD	LYS	A	97	61.884	31.343	18.578	1.00	38.30
ATOM C	727	CE	LYS	A	97	62.148	30.271	19.627	1.00	37.68
ATOM N	728	NZ	LYS	A	97	63.372	30.567	20.429	1.00	37.01
ATOM N	729	N	ASN	A	98	61.783	28.187	14.129	1.00	44.02
ATOM C	730.	CA	ASN	A	98	61.917	26.886	13.474	1.00	46.56
ATOM C	731	С	ASN	A	98	62.802	26.915	12.232	1.00	47.43
ATOM O	732	Ο.	ASN	A	98	62.605	26.126	11.307	1.00	47.95
ATOM C	733	CB	ASN	A	98	60.537	26.336	13.096	1.00	47.77
ATOM C	734	CG	ASN	Α	98	59.630	26.158	14.297	1.00	49.18
ATOM O	735	OD1	ASN	A	98	59.106	27.127	14.843	1.00	50.44
ATOM N	736	ND2	ASN	A	98	59.447	24.912	14.721	1.00	50.23
ATOM N	737	N	PHE	A	99	63.784	27.811	12.215	1.00	48.01
ATOM C	738	CA	PHE	A	99	64.676	27.927	11.068	1.00	48.77
ATOM C	739	С	PHE	Α	99	65.630	26.745	10.914	1.00	49.32
ATOM O	740	0	PHE	A	99	66.000	26.386	9.798	1.00	49.30
ATOM C	741	СВ	PHE	A	99	65.496	29.214	11.161	1.00	48.62
ATOM C	742	CG	PHE	A	99 .	66.281	29.521	9.916	1.00	48.84
ATOM C	743	CD1	PHE	A	99	65.631	29.895	8.745	1.00	48.95
ATOM C	744	CD2	PHE	A	99	67.669	29.439	9.914	1.00	49.12
ATOM C	745	CE1	PHE	A	99	66.353	30.184	7.590	1.00	49.40
ATOM C	746	CE2	PHE	A	99	68.399	29.726	8.765	1.00	48.92
ATOM C	747	CZ	PHE	A	99	67.741	30.100	7.602	1.00	49.64
ATOM N	748	N	LYS	A	100	66.032	26.147	12.031	1.00	49.95
ATOM C	749	CA	LYS	A	100	66.957	25.017	11.992	1.00.	51.02
ATOM C	750	С	LYS	A	100	66.268	23.675	11.766	1.00	51.54
	751	0	LYS	Α	100	66.911	22.628	11.824	1.00	51.71
	752	CB	LYS	A	100	67.771	24.953	13.287	1.00	51.20

ATOM C	753	CG	LYS	A	100	68.664	26.160	13.528	1.00	51.10
ATOM C	754	CD	LYS	A	100	69.464	25.986	14.808	1.00	51.19
ATOM C	755	CE	LYS	A	100	70.428	27.136	15.032	1.00	50.48
ATOM N	756	NZ	LYS	A	100	71.198	26.947	16.290	1.00	50.06
ATOM N	757	N	ALA	A	101	64.965	23.708	11.508	1.00	52.15
ATOM C	758	CA	ALA	A	101	64.201	22.486	11.272	1.00	52.52
ATOM C	759	С	ALA	Α	101	64.673	21.777	10.003	1.00	52.76
ATOM O	760	0	ALA	A	101	64.913	22.413	8.975	1.00	52.56
ATOM C	761	CB	ÀLA	A	101	62.717	22.811	11.168	1.00	52.86
ATOM N	762	· <b>N</b> .	HIS	<b>A</b>	222	79.141	30.211	17.140	1.00	53.16
ATOM C	763	CA	HIS	A	222	79.966	30.550	18.294	1.00	53.11
ATOM C	764	С	HIS	A	222	79.233	31.452	19.280	1.00	51.53
ATOM O	765	0	HIS	A	222	79.099	31.117	20.458	1.00	51.93
ATOM C	766	СВ	HIS	A	222	81.257	31.242	17.844	1.00	55.36
ATOM C	767	CG	HIS	A	222	82.390	30.299	17.582	1.00	57.46
ATOM N	768	ND1	HIS	A	222	82.940	29.508	18.568	1.00	58.71
ATOM C	769	CD2	HIS	A	222	83.087	30.032	16.452	1.00	58.36
ATOM C	770	CE1	HIS	A	222	83.928	28.794	18.056	1.00	59.17
ATOM N	771	NE2	HIS	A	222	84.038	29.093	16.774	1.00	59.10
ATOM N	772	N	ASN	A·	223	78.766	32.597	18.799	1.00	49.32
ATOM C	773	CA	ASN	A	223	78.056	33.540	19.653	1.00	47.79
ATOM C	774	C	ASN	À	223	76.565	33.582	19.357	1.00	45.63
ATOM O	775	0	ASN	A	223	75.905	34.587	19.624	1.00	44.59
ATOM C	776	CB	ASN	Α	223	78:643	34.945	19.496	1.00	49.26
ATOM ·	777	CG	ASN	A	223	80.075	35.035	19.981	1.00	50.67
ATOM O	778	OD1	ASN	A	223	80.360	34.793	21.154	1.00	51.68
ATOM N	779	ND2	ASN	Α	223	80.986	35.387	19.079	1.00	52.28
ATOM N	780	N	GLU	A	224	76.029	32.498	18.807	1.00	43.13

ATOM C	781	CA	GLU	A	224	74.606	32.467	18.503	1.00	41.15
ATOM C	782	С	GLU	A	224	73.799	32.540	19.786	1.00	38.97
ATOM O	783	0	GLU	A	224	74.153	31.927	20.792	1.00	38.56
ATOM C	784	CB	GLU	A	224	74.227	31.193	17.739	1.00	42.39
ATOM C	785	CG	GLU	A	224	74.553	29.893	18.462	1.00	44.37
ATOM C	786	CD	GLU	A	224	73.820	28.693	17.876	1.00	45.22
ATOM O	787	OE1	GLU	A	224	73.539	28.698	16.658	1.00	45.16
ATOM O	788	OE2	GLU	A	224	73.535	27.741	18.632	1.00	45.27
ATOM N	789	N	LEU	A	225	72.718	33.309	19.747	1.00	37.03
ATOM C	790	CA	LEU	A	225	71.842	33.454	20.897	1.00	36.33
ATOM C	791	С	LEU	A	225	70.674	32.500	20.682	1.00	36.34
ATOM O	792	0	LEU	A	225	69.849	32.710	19.792	1.00	34.87
ATOM C	793	СВ	LEU	Α	225	71.333	34.891	20.999	1.00	35.11
ATOM C	794	CG	LEU	A	225	70.432	35.181	22.200	1.00	34.22
ATOM C	795	CD1	LEU	A	225	71.185	34.882	23.490	1.00	34.98
ATOM C	796	CD2	LEU	A	225	69.981	36.633	22.161	1.00	33.29
ATOM N	797	N	VAL	A	226	70.608	31.453	21.500	1.00	36.84
ATOM C	798	CA	VAL	A	226	69.557	30.450	21.369	1.00	37.69
ATOM C	799	C ·	VAL	A	226	68.924	30.035	22.693	1.00	38.39
ATOM O	800	0	VAL	A	226	69.410	30.390	23.769	1.00	38.54
ATOM C	801	CB	VAL	A	226	70.108	29.174	20.702	1.00	37.69
	802	CG1	VAL	A	226	70.616	29.486	19.306	1.00	36.12
	803	CG2	VAL	A	226	71.221	28.589	21.560	1.00	38.03
	804	N	ASP	A	227	67.832	29.280	22.600	1.00	39.17
ATOM C	805	CA	ASP	A	227	67.143	28.782	23.780	1.00	39.84
	806	С	ASP	A	227	67.69 <b>7</b>	27.398	24.129	1.00	41.46
	807	0	ASP	A	227	68.671	26.944	23.526	1.00	41.37
	808	CB	ASP	A	227	65.625	28.702	23.543	1.00	39.27

ATOM C		809	CG	ASF	A	227	65.253	27.900	22.299	1.00	38.93
ATOM O		810	OD1	ASF	A	227	65.938	26.903	21.987	1.00	38.27
ATOM O		811	OD2	ASF	A	227	64.253	28.259	21.639	1.00	38.73
ATOM N		812	N	SER	A	228	67.073	26.733	25.096	1.00	42.85
ATOM C		813	CA	SER	A	228	67.510	25.408	25.535	1.00	44.79
ATOM C		814	C .	SER	Α	228	67.415	24.358	24.428	1.00	45.78
ATOM O		815	0	SER	. A	228	68.052	23.305	24.502	100	46.20
ATOM C		816	CB	SER	A	228	66.680	24.961	26.740	1.00	44.77
ATOM O		817	OG	SER	A	228	65.301	24.915	26.413	1.00	45.35
ATOM N		818	N	GLN	Α	229	66.618	24.653	23.405	1.00	46.62
ATOM C		819	CA	GLN	A	229	66.433	23.748	22.278	1.00	47,.22
ATOM C		820	С	GLN	A	229	67.327	24.128	21.102	1.00	46.93
ATOM O		821	0	GLN	A	229	67.181	23.595	20.000	1.00	46.64
ATOM C		822	CB	GLN	A	229	64.967	23.756	21.841	1.00	48.67
ATOM C		823	CG	GLN	A	229	64.029	23.082	22.828	1.00	51.08
ATOM C		824	CD	GLN	A	229	62.568	23.334	22.512	1.00	52.25
ATOM O		825	OE1	GLN	A	229	62.036	24.405	22.800	1.00	53.70
ATOM N		826	NE2	GLN	A	229	61.913	22.349	21.907	1.00	53.63
ATOM N		827	N	LYS	A	230	68.249	25.055	21.346	1.00	46.17
ATOM C		828	CA	LYS	A	230	69.188	25.512	20.324	1.00	45.18
ATOM C	ø	829	C :	LYS	A	230	68.553	26.317	19.195	1.00	43.43
ATOM O		830	0	LYS	A	230	69.146	26.471	18.126	1.00	44.02
ATOM C		831	CB	LYS	A	230	69.950	24.318	19.742	1.00	46.95
ATOM C		832	CG	LYS	A	230	70.781	23.563	20.771	1.00	48.94
ATOM C		833	CD	LYS	A	230	71.905	24.431	21.332	1.00	51.11
ATOM C		834	CE	LYS	A	230	72.929	24.788	20.257	1.00	52.17
ATOM N		835	NZ.	LYS	Α	230	74.049	25.620	20.790	1.00	53.38
ATOM N		836	N	ARG	A	231	67.353	26.836	19.429	1.00	41.91

ATOM C	837	CA	ARG	A	231	66.671	27.648	18.424	1.00	40.32
ATOM C	838	С	ARG	A	231	66.997	29.116	18.691	1.00	38.38
ATOM O	839	0	ARG	A	231	67.125	29.528	19.843	1.00	36.84
ATOM C	840	CB	ARG	A	231	65.159	27.435	18.504	1.00	42.41
ATOM C	841	CG	ARG	A	231	64.729	25.994	18.290	1.00	45.13
ATOM C	842	CD	ARG	Α	231	63.663	25.608	19.290	1.00	47.63
ATOM N	843	NE	ARG	A	231	62.397	26.291	19.050	1.00	50.64
ATOM C	844	CZ	ARG	A	231	61.549	26.636	20.013	1.00	51.82
ATOM N	845	NH1	ARG	A	231	61.842	26.371	21.277	1.00	53.05
ATOM N	846	NH2	ARG	A	231	60.401	27.230	19.712	1.00	52.91
ATOM N	847	·N	TYR	A	232	67.140	29.896	17.627	1.00	36.74
ATOM C	848	CA	TYR	Α	232	67.451	31.313	17.763	1.00	35.61
ATOM C	849	С	TYR	A	232	66.388	32.035	18.579	1.00	34.70
ATOM O	850	0	TYR	Α	232	65.193	31.755	18.453	1.00	33.91
ATOM C	851	CB	TYR	A	232	67.538	31.976	16.390	1.00	36.14
ATOM C	852	CG	TYR	A	232	68.648	31.455	15.517	1.00	37.40
ATOM C	853	CD1	TYR	A	232	69.973	31.464	15.955	1.00	37.55
ATOM C	854	CD2	TYR	A	232	68.377	30.966	14.241	1.00	38.07
ATOM C	855	CE1	TYR	A	232	71.003	30.996	15.136	1.00	39.02
ATOM C	856	CE2	TYR	A	232	69.396	30.498	13.419	1.00	39.05
ATOM C	857	CZ	TYR	A	232	70.703	30.516	13.870	1.00	39.19
ATOM O	858	ОН	TYR	A	232	71.704	30.060	13.045	1.00	40.49
ATOM N	859	N	LEU	A	233	66.823	32.964	19.420	1.00	33.09
ATOM C	860	CA	LEU	A	233	65.877	33.726	20.214	1.00	32.70
ATOM C	861	С	LEU	A	233	65.359	34.854	19.338	1.00	31.76
ATOM O	862	0	LEU	A	233	66.051	35.321	18.431	1.00	32.09
ATOM C	863	СВ	LEU	A	233	66.541	34.310	21.467	1.00	32.69
ATOM C	864	CG	LEU	Α	233	67.114	33.357	22.522	1.00	33.44

ATOM C	865	CD1	LEU	A	233		67.532	34.178	23.738	1.00 33.23
ATOM C	866	CD2	LEU	A	233		66.084	32.316	22.936	1.00 33.22
ATOM N	867	N	VAL	A	234		64.132	35.281	19.598	1.00 32.10
ATOM C	868	CA	VAL	A	234		63.539	36.365	18.839	1.00 31.38
ATOM C	869	С	VAL	A	234		62.535	37.088	19.723	1.00 30.84
ATOM O	870	0	VAL	A	234		61.919	36.487	20.601	1.00 30.80
ATOM C	871	СВ	VAL	A	234		62.832	35.845	17.560	1.00 31.94
ATOM C	872	CG1	VAL	A	234		61.608	35.011	17.930	1.00 31.25
ATOM C	873	CG2	VAL	A	234		62.448	37.013	16.672	1.00 30.99
ATOM N	874	N	GLY	A	235		62.400	38.391	19.508	1.00 30.91
ATOM C	875	CA	GLY	A	235		61.456	39.164	20.286	1.00 30.22
ATOM C	876	С	GLY	A	235		60.382	39.673	19.349	1.00 29.78
ATOM O	877	0	GLY	A	235		60.501	39.517	18.136	1.00 29.75
ATOM N	878	N	ALA	A	236		59.336	40.276	19.904	1.00 29.91
ATOM C	879	CA	ALA	A	236		58.255	40.811	19.093	1.00 29.86
ATOM C	880	С	ALA	A	236		57.639	42.027	19.774	1.00 29.27
ATOM O	881	0	ALA	A	236		57.439	42.037	20.986	1.00 29.23
ATOM C	882	CB	ALA	A	236	,	57.192	39.741	18.868	1.00 30.79
ATOM N	883	N	GLY	A	237		57.345	43.054	18.987	1.00 29.87
ATOM C	884	CA	GLY	A	237		56.745	44.249	19.544	1.00 29.77
ATOM C	885	С	GLY	A	237		55.242	44.109	19.649	1.00 30.45
ATOM O	886	0	GLY	A	237		54.626	43.420	18.839 ·	1.00 30.39
ATOM N	887	И	ILE	A	238		54.650	44.744	20.656	1.00 29.85
ATOM C	888	CA	ILÉ	A	238		53.206	44.703	20.835	1.00 30.46
ATOM C	889	С	ILE	A	238		52.708	46.115	21.130	1.00 31.10
ATOM O	890	0	ILE .	A	238		53.493	47.003	21.470	1.00 30.41
	891	СВ	ILE .	A.	238		52.788	43.767	22.001	1.00 29.94
ATOM C	892	CG1	ILE .	A :	238		53.310	44.313	23.333	1.00 30.64

ATOM C	893	CG2	ILE	A	238	53.322	42.357	21.758	1.00	29.80
ATOM C	894	CD1	ILE	A	238	52.808	43.550	24.556	1.00	31.03
ATOM N	895	N	ASN	A	239	51.406	46.328	20.980	1.00	31.30
ATOM C	896	CA.	ASN	A	239	50.825	47.632	21.249	1.00	30.86
ATOM C	897	С	ASN	Α	239	49.859	47.518	22.419	1.00	31.81
ATOM O	898	0	ASN	A	239	49.535	46.416	22.862	1.00	30.42
ATOM C	899	СВ	ASN	A	239	50.108	48.171	20.006	1.00	31.76
ATOM C	900	CG	ASN	A	239	49.028	47:231	19.495	1.00	31.45
ATOM O	901	OD1	ASN	A	239	48.019	47.004	20.160	1.00	32.62
ATOM N	902	ND2	ASN	A	239	49.240	46.678	18.309	1.00	32.41
ATOM .	903	N	THR	A	240	49.406	48.660	22.921	1.00	32.10
ATOM C	904	CA	THR	A	240	48.494	48.686	24.054	1.00	32.56
ATOM C	905	С	THR	A	240	47.025	48.523	23.648	1.00	34.33
ATOM O	906	0	THR	A	240	46.130	48.681	24.477	1.00	33.93
ATOM C	907	CB	THR	A	240	48.653	50.004	24.831	1.00	32.45
ATOM O	908	OG1	THR	A	240	48.432	51.107	23.941	1.00	31.46
ATOM C	909	CG2	THR	A	240	50.065	50.112	25.418	1.00	31.19
ATOM N	910	N	ARG	A	241	46.787	48.179	22.385	1.00	35.96
ATOM C	911	ÇA	ARG	A	241	45.426	48.032	21.873	1.00	39.04
	912	С	ARG	A	241	44.919	46.596	21.719	1.00	39.35 [°]
	913	0	ARG	A	241	43.981	46.188	22.406	1.00	40.01
	914	СВ	ARG	A	241	45.313	48.743	20.522	1.00	41.18
	915	CG	ARG	A	241	45.852	50.167	20.516	1.00	45.22
	916	CD	ARG	A	241	44.809	51.195	20.920	1.00	48.22
ATOM N	917	NE	ARG	A	241	43.702	51.247	19.968	1.00	50.77
ATOM C	918	CZ	ARG	Α	241	42.962	52.329	19.735	1.00	52.50
	919	NHl	ARG	A	241	43.211	53.461	20.383	1.00	52.88
	920	NH2	ARG	A	241	41.971	52.279	18.853	1.00	52.52

ATOM N	921	N	ASP	A	242	45.532	45.836	20.816	1.00	39.54
ATOM C	922	CA	ASP	A	242	45.105	44.459	20.557	1.00	40.21
ATOM C	923	С	ASP	A	242	45.938	43.371	21.230	1.00	39.85
ATOM O	924	0	ASP	A	242	46.016	42.253	20.723	1.00	40.56
ATOM C	925	CB	ASP	A	242	45.087	44.192	19.045	1.00	40.36
ATOM C	926	CG	ASP	A	242	46.461	44.345	18.399	1.00	40.93
ATOM O	927	OD1	ASP	A	242	47.480	44.013	19.045	1.00	41.17
ATOM O	928	OD2	ASP	A	242	46.526	44.781	17.230	1.00	41.45
ATOM N	929	N	PHE	A	243	46.537	43.681	22.373	1.00	39.48
ATOM C	930	CA	PHE	A	243	47.381	42.712	23.066	1.00	39.13
ATOM C	931	С	PHE	A	243	46.677	41.442	23.547	1.00	39.39
ATOM O	932	0	PHE	A	243	47.293	40.380	23.604	1.00	38.77
ATOM C	933	CB	PHE	A	243	48.108	43.392	24.235	1.00	37.88
ATOM C	934	CG	PHE	Α	243	47.198	43.915	25.305	1.00	37.59
ATOM C	935	CD1	PHE	A	243	46.746	43.082	26.323	1.00	37.35
ATOM C	936	CD2	PHE	A	243	46.797	45.248	25.301	1.00	37.10
AŢOM C	937	CE1	PHE	A	243	45.908	43.569	27.326	1.00	37.14
ATOM C	938	CE2	PHE	A	243	45.959	45.744	26.299	1.00	37.25
ATOM C	939	CZ	PHE	Α	243	45.515	44.901	27.313	1.00	37.29
ATOM N	940	N	ARG	A	244	45.395	41.543	23.887	1.00	40.11
ATOM C	941	CA	ARG	A	244	44.653	40.375	24.354	1.00	40.93
ATOM C	942	С	ARG	A	244	44.619	39.281	23.289	1.00	40.69
	943	0	ARG	A	244	44.502	38.099	23.609	1.00	41.20
ATOM C	944	CB	ARG	A	244 .	43.229	40.773	24.760	1.00	41.45
ATOM C	945	CG	ARG	Α	244	43.188	41.719	25.952	1.00	42.10
ATOM C	946	CD	ARG	A	244	41.766	42.050	26.382	1.00	43.32
ATOM N	947	NE	ARG	Α	244	41.749	43.039	27.456	1.00	44.43
ATOM C	948	CZ	ARG	A	244	42.035	44.328	27.291	1.00	45.14

ATOM N	949	NH1	ARG	A	244	42.357	44.793	26.090	1.00	44.75
ATOM N	950	NH2	ARG	A	244	42.010	45.153	28.329	1.00	45.44
MOTA	951	N	GLU	A	245	44.726	39.677	22.026	1.00	40.84
N ATOM C	952	CA	GLU	A	245	44.732	38.718	20.928	1.00	40.87
ATOM C	953	С	GLU	A	245	46.147	38.501	20.393	1.00	40.07
ATOM O	954	0	GLU	A	245	46.537	37.374	20.083	1.00	39.45
ATOM C	955	CB	GLU	A	245	43.838	39.197	19.781	1.00	43.54
ATOM C	956	CG	GLU	A	245	42.334	39.160	20.061	1.00	47.70
ATOM C	957	CD	GLU	Α	245	41.900	40.111	21.164	1.00	50.68
ATOM O	958	OE1	GLU	A	245	42.282	41.305	21.121	1.00	52.80
ATOM O	959	OE2	GLU	A	245	41.162	39.665	22.072	1.00	52.45
ATOM N	960	N	ARĠ	A	246	46.915	39.581	20.291	1.00	38.14
ATOM C	961	CA	ARG	A	246	48.277	39.501	19.764	1.00	36.50
ATOM C	962	С	ARG	A	246	49.259	38.743	20.660	1.00	36.05
ATOM O	963	0	ARG	A	246	50.051	37.943	20.170	1.00	36.35
ATOM	964	CB	ARG	A	246	48.814	40.913	19.489	1.00	35.90
C ATOM C	965	CG	ARG	A	246 .	50.130	40.945	18.713	1.00	35.45
ATOM C	966	CD	ARG	A	246	50.611	42.375	18.505	1.00	34.86
ATOM N	967	NE	ARG	A	246.	49.743	43.147	17.619	1.00	34.95
ATOM C	968	CZ	ARG	A	246	49.766	43.077	16.291	1.00	34.35
ATOM N	969	NHl	ARG	A	246	50.616	42.267	15.676	1.00	35.15
ATOM N	970	NH2	ARG	A	246	48.939	43.827	15.574	1.00	35.50
ATOM N	971	N	VAL	A	247	49.212	38.986	21.967	1.00	35.97
ATOM C	972	CA	VAL	A	247	50.129	38.315	22.886	1.00	36.75
ATOM C	973	С	VAL	A	247	50.020	36.788	22.837	1.00	37.56
ATOM O	974	0	VAL	A	247	51.033	36.096	22.706	1.00	37.16
ATOM C	975	CB	VAL	A	247	49.927	38.806	24.340	1.00	36.31
ATOM C	976	CG1	VAL	A	247	50.775	37.987	25.296	1.00	35.75

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ATOM C	977	CG2	VAL	A	247	50.314	40.282	24.444	1.00	36.50
ATOM N	978	N .	PRO	A	248	48.794	36.241	22.946	1.00	37.33
ATOM C	979	CA	PRO	A	248	48.638	34.783	22.901	1.00	36.95
ATOM C	980	C	PRO	A	248	49.231	34.184	21.629	1.00	36.36
ATOM O	981	0	PRO	A	248	49.897	33.155	21.677	1.00	37.14
ATOM C	982	CB	PRO	A	248	47.125	34.598	22.979	1.00	37.52
ATOM C	983	CG	PRO	A	248	46.709	35.735	23.858	1.00	37.69
ATOM C	984	CD	PRO	A	248	47.515	36.890	23.290	1.00	36.69
ATOM N	985	N	ALA	A	249	48.997	34.840	20.497	1.00	35.60
ATOM C	986	CA	ALA	A	249	49.507	34.367	19.217	1.00	35.36
ATOM C	987	С	ALA	A	249	51.034	34.354	19.183	1.00	35.63
ATOM O	988	0	ALA	A	249	51.646	33.411	18.669	1.00	33.65
ATOM C	989	CB	ALA	A	249	48.968	35.236	18.090	1.00	36.03
ATOM N	990	N	LEU	Α	250	51.646	35.403	19.728	1.00	35.24
ATOM C	991	CA	LEU	A	250	53.099	35.505	19.754	1.00	35.85
ATOM C	992	С	LEU	A	250	53.701	34.458	20.681	1.00	36.48
ATOM O	993	0	LEU	A	250	54.758	33.899	20.395	1.00	36.97
ATOM C	994	CB	LEU	A	250	53.520	36.915	20.189	1.00	34.62
ATOM C	995	CG	LEU	A	250	53.067	38.010	19.215	1.00	34.74
ATOM C	996	CD1	LEU	A	250	53.473	39.384	19.731	1.00	34.92
ATOM C	997	CD2	LEU	. <b>A</b>	250	53.678	37.749	17.847	1.00	34.43
ATOM N	998	N	VAL	A	251	53.025	34.191	21.790	1.00	38.25
ATOM C	999	CA	VAL	A	251	53.501	33.193	22.738	1.00	40.28
ATOM C	1000	С	VAL	A	251	53.471	31.810	22.087	1.00	41.33
ATOM O	1001	0	VAL	Α	251	54.447	31.062	22.159	1.00	41.27
ATOM .C	1002	СВ	VAL	A	251	52.632	33.173	24.013	1.00	40.67
ATOM C	1003	CG1	VAL	A	251	53.018	31.986	24.895	1.00	42.14
ATOM C	1004	CG2	VAL	A	251	52.813	34.474	24.780	1.00	40.95

ATOM N	1005	N	GLU	A	252	52.355	31.480	21.439	1.00	41.97
ATOM C	1006	CA	GLU	A	252	52.217	30.182	20.783	1.00	43.27
ATOM C	1007	С	GLU	A	252	53.252	30.030	19.679	1.00	42.06
ATOM O	1008	0	GLU	A	252	53.804	28.949	19.484	1.00	42.29
ATOM C	1009	CB	GLU	A	252	50.822	30.019	20.172	1.00	45.54
ATOM C	1010	CG	GLU	A	252	49.688	30.558	21.016	1.00	49.93
ATOM C	1011	CD	GLU	A	252	49.586	29.929	22.392	1.00	52.52
ATOM O	1012	OE1	GLU	A	252	48.789	30.449	23.201	1.00	54.25
ATOM O	1013	OE2	GLU	A	252	50.280	28.924	22.670	1.00	55.02
ATOM N	1014	N	ALA	Α	253	53.503	31.116	18.953	1.00	40.26
ATOM C	1015	CA	ALA	A	253	54.472	31.103	17.865	1.00	38.87
ATOM C	1016	С	ALA	A	253	55.889	30.880	18.390	1.00	38.28
ATOM O	1017	0	ALA	A	253	56.788	30.523	17.628	1.00	38.29
ATOM C	1018	CB	ALA	A	253	54.398	32.406	17.082	1.00	39.08
ATOM N	1019	N	GLY	A	254	56.088	31.103	19.686	1.00	37.14
ATOM C	1020	CA	GLY	A	254	57.399	30.885	20.275	1.00	36.67
ATOM C	1021	С	GLY	Α	254	58.226	32.111	20.631	1.00	35.76
ATOM O	1022	0	GLY	A	254	59.433	31.995	20.845	1.00	35.05
ATOM N	1023	N	ALA	A	255	57.596	33.282	20.701	1.00	35.10
ATOM C	1024	CA	ALA	A	255	58.321	34.502	21.045	1.00	34.05
ATOM C	1025	C	ALA	A	255	59.011	34.342	22.399	1.00	33.03
ATOM O	1026				255			23.372	1.00	32.76
ATOM C	1027				255			21.078		34.00
ATOM N	1028	Ν .	ASP	A	256	60.285	34.710	22.454	1.00	32.35
ATOM C	1029				256			23.682	1.00	32.05
ATOM C	1030				256			24.597	1.00	31.18
ATOM O	1031	0	ASP	A	256	61.004	35.699	25.817	1.00	30.47
ATOM C	1032	CB	ASP .	A	256	62.531	34.409	23.329	1.00	32.35

ATOM C	1033	CG	ASP	A	256	62.770	33.118	22.575	1.00	34.08
ATOM O	1034	OD1	ASP	A	256	62.639	32.044	23.199	1.00	34.90
ATOM O	1035	OD2	ASP	A	256	63.068	33.172	21.365	1.00	33.17
ATOM N	1036	N	VAL	A	257	60.602	36.957	24.002	1.00	30.50
ATOM C	1037	CA	VAL	A	257	60.402	38.173	24.778	1.00	29.68
ATOM C	1038	C	VAL	A	257	59.555	39.139	23.961	1.00	29.30
ATOM O	1039	0	VAL	A	257	59.584	39.111	22.733	1.00	29.73
ATOM C	1040	CB	VAL	A	257	61.756	38.844	25.125	1.00	29.48
ATOM C	1041	CG1	VAL	A	257	62.462	39.273	23.848	1.00	29.83
ATOM C	1042	CG2	VAL	A	257	61.531	40.040	26.044	1.00	29.61
ATOM N	1043	N	LEU	A	258	58.800	39.982	24.654	1.00	28.19
ATOM C	1044	CA	LEU	A	258	57.942	40.961	24.007	1.00	28.90
ATOM C	1045	С	LEU	A	258	58.369	42.354	24.457	1.00	28.21
ATOM O	1046	0	LEU	A	258	59.113	42.503	25.419	1.00	28.37
ATOM C	1047	CB	LEU	A	258	56.485	40.746	24.425	1.00	27.71
ATOM C	1048	CG	LEU	A	258	55.915	39.332	24.289	1.00	28.73
ATOM C	1049	CD1	LEU	A	258	54.508	39.297	24.871	1.00	30.02
ATOM C .	1050	CD2	LEU	A	258	55.907	38.917	22.833	1.00	29.49
ATOM N	1051	N	CYS	A	259	57.898	43.373	23.754	1.00	28.75
	1052	CA	CYS	A	259	58.206	44.743	24.142	1.00	28.59
ATOM C	1053	С	CYS	A	259	57.122	45.669	23.617	1.00	28.15
ATOM O	1054	0	CYS	A	259	56.827	45.670	22.423	1.00	28.23
ATOM C	1055	CB	CYS	A	259	59.566	45.181	23.597	1.00	28.11
ATOM S	1056	SG	CYS	A	259	60.079	46.808	24.215	1.00	29.44
ATOM N	1057	N	ILE	A	260	56.525	46.443	24.518	1.00	28.54
ATOM C	1058	CA	ILE	A	260	55.490	47.392	24.132	1.00	29.64
ATOM C	1059	C	ILE	A	260	56.191	48.503	23.362	1.00	30.85
ATOM O	1060	0	ILE	A	260	57.144	49.106	23.852	1.00	30.69

ATOM C	1061	CB	ILE	A	260	54.786	47.985	25.361	1.00	29.60
ATOM C	1062	CG1	ILE	A	260	54.254	46.849	26.238	1.00	29.82
ATOM C	1063	CG2	ILE	A	260	53.638	48.901	24.916	1.00	29.89
ATOM C	1064	CD1	ILE	A	260	53.659	47.309	27.557	1.00	30.44
ATOM N	1065	N	ASP	Α	261	55.702	48.760	22.156	1.00	31.00
ATOM C	1066	CA	ASP	A	261	56.266	49.756	21.257	1.00	32.38
ATOM C	1067	С	ASP	Ą	261	55.498	51.081	21.316	1.00	32.90
ATOM O	1068	0	ASP	A	261	54.361	51.162	20.859	1.00	32.73
ATOM C	1069	CB	ASP	Α	261	56.252	49.151	19.846	1.00	33.58
ATOM C	1070	CĠ	ASP	A	261	56.773	50,088	18.783	1.00	35.13
ATOM O	1071	OD1	ASP	A	261	57.544	51.012	19.104	1.00	35.01
ATOM O	1072	OD2	ASP	A	261	56.415	49.874	17.604	1.00	35.63
ATOM N	1073	N	SER	A	262	56.121	52.112	21.888	1.00	32.69
ATOM C	1074	CA	SER	A	262	55.483	53.427	22.013	1.00	32.90
ATOM C	1075	С	SER	A	262	56.502	54.557	22.175	1.00	32.98
ATOM O	1076	0	SER	A	262	57.598	54.339	22.686	1.00	32.40
ATOM C	1077	CB	SER	A	262	54.529	53.423	23.213	1.00	33.69
ATOM O	1078	OG .	SER	A	262	54.010	54.716	23.469	1.00	35.09
ATOM N	1079	N	SER	A	263	56.142	55.766	21.745	1.00	32.80
ATOM ·	1080	CA	SER	A	263	57.0 <u>4</u> 8	56.906	21.872	1.00	33.15
ATOM C	1081	С	SER	A	263	56.985	57.508	23.276	1.00	33.32
ATOM O	1082	0	SER	A	263	57.932	58.151	23.722	1.00	35.72
ATOM C	1083	СВ	SER	A	263	56.734	57.976	20.816	1.00	34.60
ATOM O	1084	OG	SER	Α	263	55.370	58.352	20.845	1.00	37.69
ATOM N	1085	N	ASP	A	264	55.871	57.296	23.971	1.00	31.32
ATOM C	1086	CA	ASP	A	264	55.711	57.795	25.337	1.00	29.82
ATOM C	1087	С	ASP	A	264	55.158	56.664	26.203	1.00	29.45
ATOM O	1088	0	ASP	A	264	53.942	56.475	26.304	1.00	28.91

ATOM C	1089	CB	ASP	A	264	54.775	59.017	25.356	1.00	28.89
ATOM C	1090	CG	ASP	A	264	54.352	59.436	26.769	1.00	29.68
ATOM O	1091	OD1	ASP	A	264	55.007	59.067	27.768	1.00	26.79
ATOM O	1092	OD2	ASP	A	264	53.348	60.168	26.877	1.00	29.53
ATOM N	1093	N	GLY	A	265	56.071	55.914	26.815	1.00	27.82
ATOM C	1094	CA	GLY	A	265	55.692	54.796	27.662	1.00	27.73
ATOM C	1095	·C	GLY	A	265	55.189	55.151	29.048	1.00	27.21
ATOM O	1096	0	GLY	A	265	54.751	54.269	29.784	1.00	27.06
ATOM N	1097	N	PHE	A	266	55.244	56.430	29.412	1.00	26.33
ATOM C	1098	CA	PHE	A	266	54.779	56.870	30.726	1.00	26.29
ATOM C	1099	С	PHE	A	266	53.265	56.989	30.574	1.00	27.35 ⁻
ATOM O	1100	0	PHE	A	266	52.707	58.086	30.516	1.00	26.16
ATOM C	1101	CB	PHE	A	266	55.403	58.222	31.071	1.00	26.18
ATOM C	1102	CG	PHE	A	266	55.499	58.503	32.553	1.00	27.83
ATOM C	1103	CD1	PHE	A	266	54.770	57.754	33.481	1.00	26.01
ATOM C	1104	CD2	PHE	A	266	56.305	59.541	33.017	1.00	26.81
ATOM C	1105	CE1	PHE	A	266	54.846	58.040	34.843	1.00	27.31
ATOM C	1106	CE2	PHE	A	266,	56.385	59.833	34.373	1.00	27.03
ATOM . C	1107	CZ	PHE	A	266	55.654	59.081	35.291	1.00	27.65
ATOM N	1108	N	SER	A	267	52.613	55.832	30.502	1.00	28.62
ATOM C	1109	CA	SER	A	267	51.176	55.751	30.282	1.00	29.12
ATOM C	1110	С	SER	A	267	50.490	54.634	31.061	1.00	29.52
ATOM O	1111	0	SER	A	267	51.036	53.543	31.231	1.00	27.59
ATOM C	1112	CB	SER	A	267	50.924	55.535	28.790	1.00	30.27
ATOM O	1113	OG	SER	A	267	49.593	55.132	28.534	1.00	33.40
ATOM N	1114	N	GLU	A	268	49.272	54.912	31.507	1.00	30.01
ATOM C	1115	CA	GLU	A	268	48.493	53.936	32.246	1.00	31.53
ATOM C	1116	С	GLU	A	268	48.208	52.753	31.328	1.00	31.63

ATOM O	1117	0	GLU	Α	268	48.000	51.627	31.790	1.00	31.90
ATOM C	1118	СВ	GLU	Α	268	47.184	54.572	32.716	1.00	33.65
ATOM C	1119	CG	GLU	A	268	46.385	53.720	33.684	1.00	36.92
ATOM C	1120	CD	GLU	A	268	45.169	54.445	34.238	1.00	38.90
ATOM O	1121	OE1	GLU	A	268	44.448	53.837	35.059	1.00	41.93
ATOM O	1122	OE2	GLU	Α	268	44.933	55.615	33.857	1.00	37.65
ATOM N	1123	N	TRP	A	269 -	48.212	53.007	30.022	1.00	30.66
ATOM C	1124	CA	TRP	Α	269	47.960	51.950	29.053	1.00	32.73
ATOM C	1125	С	TRP	A	269	49.023	50.858	29.122	1.00	31.60
ATOM O	1126	0	TRP	A	269	48.717	49.678	28.951	1.00	32.00
ATOM C	1127	CB	TRP	A	269 ·	47.890	52.520	27.632	1.00	34.13
ATOM C	1128	CG	TRP	A	269	46.705	53.411	27.401	1.00	38.84
ATOM	1129	CD1	TRP	A	269	46.723	54.759	27.170	1.00	39.63
C ATOM C	1130	CD2	TRP	Å	269	45.325	53.021	27.383	1.00	40.48
ATOM N	1131	NE1	TRP	A	269	45.442	55.229	27.009	1.00	40.70
MOTA	1132	CE2	TRP	A	269	44.565	54.185	27.134	1.00	40.74
C ATOM C	1133	CE3	TRP	A	269	44.657	51.800	27.553	1.00	41.39
ATOM C	1134	CZ2	TRP	A	269	43.168	54.165	27.049	1.00	42.44
ATOM C	1135	CZ3	TRP	A	269	43.266	51.780	27.469	1.00	42.63
ATOM C	1136	CH2	TRP	A	269	42.539	52.957	27.219	1.00	42.95
ATOM N	1137	N	GLN	A	270	50.273	51.237	29.370	1.00	30.36
MOTA	1138	CA	GLN	A	270	51.330	50.232	29.463	1.00	29.91
C ATOM C	1139	С	GLN	A	270	51.197	49.444	30.764	1.00	29.40
MOTA O	1140	0	GLN	A	270	51.478	48.250	30.802	1.00	29.26
ATOM C	1141	СВ	GLN	A	270	52.717	50.883	29.369	1.00	28.96
MOTA	1142	CG	GLN	A	270	52.925	51.642	28.065	1.00	28.77
C ATOM C	1143	CD	GLN	Α	270	54.293	51.420	27.438	1.00	28.29
ATOM O	1144	OE1	GLN	Α	270	55.185	50.820	28.041	1.00	27.12

ATOM N	1145	NE2	GLN	A	270	54.463	51.916	26.217	1.00	26.63
ATOM N	1146	<b>N</b> .	LYS	A	271	50.763	50.113	31.828	1.00	30.02
ATOM C	1147	CA	LYS	A	271	50.579	49.437	33.107	1.00	31.43
ATOM C	1148	C .	LYS	A	271	49.484	48.381	32.944	1.00	31.09
ATOM O	1149	0	LYS	A	271	49.618	47.257	33.419	1.00	30.76
ATOM C	1150	CB	LYS	A	271 .	50.181	50.433	34.202	1.00	33.38
ATOM [.]	1151	CG	LYS	A	271	49.911	49.770	35.552	1.00	36.04
ATOM C	1152	CD	LYS	A	271	49.607	50.779	36.655	1.00	37.85
ATOM C	1153	CE	LYS	A	271	49.404	50.068	37.993	1.00	40.25
ATOM N	1154	NZ	LYS	A	271	49.157	51.008	39.131	1.00	42.83
ATOM N	1155	N	ILE	A	272	48.409	48.752	32.257	1.00	31.55
ATOM C	1156	CA	ILE	A	272	47.291	47.841	32.018	1.00	31.85
ATOM C	1157	С	ILE	A	272	47.745	46.632	31.202	1.00	31.95
ATOM O	1158	0	ILE	A	272	47.433	45.490	31.544	1.00	31.04
ATOM C	1159	CB	ILE	A	272	46.139	48.565	31.278	1.00	31.97
ATOM C	1160	CG1	ILE	A	272	45.463	49.551	32.235	1.00	32.25
ATOM C	1161	CG2	ILE	A	272	45.137	47.552	30.730	1.00	32.38
ATOM C	1162	CD1	ILE	Α	272	44.456	50.473	31.570	1.00	32.51
ATOM N	1163	N	THR	A	273	48.492	46.890	30.133	1.00	30.63
ATOM C	1164	CA	THR	A	273	48.995	45.833	29.267	1.00	31.00
ATOM C	1165	C	THR	A	273	49.882	44.849	30.030	1.00	31.56
ATOM O	1166	0	THR	Α	273	49.702	43.633	29.927	1.00	31.43
ATOM C	1167	CB	THR	A	273	49.796	46.422	28.084	1.00	30.85
ATOM O	1168	OG1	THR	A	273	48.932	47.244	27.292	1.00	32.26
ATOM C	1169	CG2	THR	A	273	50.366	45.311	27.208	1.00	30.97
ATOM N	1170	N	ILE	A	274	50.843	45.370	30.789	1.00	31.51
	1171	CA	ILE	A	274	51.736	44.506	31.558	1.00	32.20
	1172	С	ILE	A	274	50.927	43.738	32.603	1.00	32.56

ATOM O	1173	0	ILE	A	274	51.189	42.566	32.870	1.00	32.30
ATOM C	1174	CB	ILE	A	274	52.825	45.314	32.288	1.00	31.42
ATOM C	1175	CG1	ILE	A	274	53.653	46.114	31.278	1.00	32.15
ATOM C	1176	CG2	ILE	A	274	53.718	44.367	33.091	1.00	31.67
ATOM C	1177	CD1	ILE	A	274	54.655	47.065	31.920	1.00	32.30
ATOM N	1178	N	GLY	A	275	49.941	44.410	33.189	1.00	32.77
ATOM C	1179	CA	GLY	A	275	49.110	43.775	34.196	1.00	33.56
ATOM C	1180	С	GLY	A	275	48.351	42.578	33.653	1.00	34.04
ATOM O	1181	0	GLY	A	275	48.245	41.546	34.320	1.00	34.05
ATOM ·	1182	N	TRP	A	276	47.822	42.714	32.443	1.00	33.68
ATOM C	1183	CA	TRP	A	276	47.065	41.642	31.⁄804	1.00	34.90
ATOM C	1184	C	TRP	A	276	47.980	40.451	31.536	1.00	35.94
ATOM O	1185	0	TRP	A	276	47.581	39.293	31.700	1.00	34.92
ATOM C	1186	CB	TRP	A	276	46.469	42.134	30.485	1.00	35.21
ATOM C	1187	CG	TRP	Α	276	45.582	41.138	29.813	1.00	36.07
ATOM C	1188	CD1	TRP	Α	276	44.237	40.972	30.002	1.00	36.67
ATOM C	1189	CD2	TRP	A	276	45.978	40.153	28.853	1.00	36.84
ATOM N	1190	NE1	TRP	A	276	43.772	39.944	29.212	1.00	36.48
ATOM C	1191	CE2	TRP	A	276	44.820	39.424	28.498	1.00	37.06
ATOM C	1192	CE3	TRP	Ą	276	47.201	39.814	28.255	1.00.	36.59
ATOM C	1193	CZ2	TRP	A	276	44.848	38.376	27.572	1.00	37.28
ATOM C	1194	CZ3	TRP	A	276	47.230	38.772	27.336	1.00	37.26
ATOM C	1195	CH2	TRP	A	276	46.057	38.065	27.004	1.00	37.96
ATOM N	1196	N	ILE	A	277	49.211	40.740	31.121	1.00	35.54
ATOM C	1197	CA	ILE	A	277	50.181	39.690	30.835	1.00	36.20
ATOM C	1198	С	ILE	A	277	50.562	38.933	32.109	1.00	37.31
ATOM O	1199	0	ILE	A	277	50.646	37.703	32.106	1.00	37.04
ATOM C	1200	CB	ILE	A	277	51.456	40.279	30.178	1.00	35.46

ATOM C	1201	CG1	ILE	A	277	51.112	40.828	28.791	1.00	35.23
ATOM C	1202	CG2	ILE	A	277	52.541	39.210	30.080	1.00	35.59
ATOM C	1203	CD1	ILE	A	277	52.273	41.503	28.081	1.00	35.42
MOTA N	1204	N	ARG	A	278	50.787	39.666	33.194	1.00	38.07
ATOM C	1205	CA	ARG	A	278	51.152	39.047	34.466	1.00	39.93
ATOM C	1206	С	ARG	Α	278	50.029	38.167	35.005	1.00	41.35
ATOM ·	1207	0	ARG	A	278	50.273	37.077	35.517	1.00	41.11
ATOM C	1208	CB	ARG	A	278	51.489	40.120	35.502	1.00	39.44
ATOM C	1209	CG	ARG	A	278	52.797	40.835	35.243	1.00	38.20
ATOM C	1210	CD.	ARG	Α	278	53.989	39.927	35.511	1.00	38.69
ATOM N	1211	NE	ARG	A	278	55.225	40.567	35.075	1.00	37.38
ATOM C	1212	CZ	ARG	A	278	55.937	40.181	34.023	1.00	37.01
ATOM N	1213	NH1	ARG	A	278	55.547	39.141	33.297	1.00	35.28
ATOM N	1214	NH2	ARG	A	278	57.022	40.861	33.674	1.00	34.80
ATOM N	1215	N	GLU	A	279	48.801	38.654	34.891	1.00	42.82
ATOM	1216.	CA	GLU	A	279	47.634	37.922	35.369	1.00	45.18
C ATOM C	1217	С	GLU	A	279	47.353	36.655	34.559	1.00	45.03
ATOM O	1218	0	GLU	Α	279	46.793	35.686	35.076	1.00	45.43
ATOM C	1219	CB	GLU	A	279	46.417	38.858	35.355	1.00	47.47
ATOM C	1220	CG	GLU	A	279	45.058	38.180	35.269	1.00	51.44
ATOM C	1221	CD	GLU	A	279	44.757	37.662	33.873	1.00	53.84
ATOM	1222	OE1	GLU	A	279	44.818	38.465	32.909	1.00	54.89
O ATOM O	1223	OE2	GLU	A	279	44.460	36.454	33.740	1.00	54.90
ATOM N	1224	N	LYS	A	280	47.755	36.655	33.294	1.00	44.19
ATOM C	1225	CA	LYS	A	280	47.513	35.515	32.421	1.00	43.85
ATOM C	1226	С	LYS	A	280	48.704	34.558	32.319	1.00	43.09
ATOM O	1227	0	LYS	A	280	48.523	33.356	32.109	1.00	42.03
ATOM C	1228	CB	LYS	A	280	47.133	36.030	31.027	1.00	45.44

ATOM C	1229	CG	LYS	A	280	46.346	35.059	30.153	1.00	48.33
ATOM C	1230	CD	LYS	A	280	47.213	33.959	29.575	1.00	50.41
ATOM	1231	CE	LYS	A	280	46.394	33:011	28.702	1.00	51.95
C ATOM N	1232	NZ	LYS	Α	280	45.734	33.714	27.563	1.00	52.39
ATOM N	1233	N	TYR	A	281	49.915	35.082	32.494		41.24
ATOM	1234	CA	TYR	A	281	51.121	34.268	32.369	1.00	39.92
C ATOM C	1235	С	TYR	A	281	52.095	34.338	33.535	1.00	39.29
ATOM O	1236	0	TYR	A	281	53.103	33.636	33.538	~	38.90
MOTA	1237	СВ	TYR	A	281	51.882	34.674	31.110	1.00	40.32
C ATOM C	1238	CG	TYR	A	281	51.108	34.542	29.823	1.00	40.12
ATOM C	1239	CD1	TYR	A	281	50.920	33.296	29.224		40.31
ATOM	1240	CD2	TYR	A	281	50.595	35.668	29.181	1.00	40.13
C ATOM	1241	CE1	TYR	A	281	50.246	33.178	28.013	1.00	40.79
C ATOM C	1242	CE2	TYR	A	281	49.918	35.560	27.973	1.00	40.17
ATOM C	1243	CZ	TYR	Α	281	49.750	34.314	27.393	1.00	41.11
MOTA	1244	OH	TYR	A	281	49.097	34.208	26.188	1.00	41.85
O ATOM N	1245	N	GLY	A	282	51.812	35.181	34.517	1.00	38.90
ATOM C	1246	CA	GLY	A	282	52.733	35.306	35.629		39.41
ATOM	1247	С	GLY	A	282	54.044	35.871	35.105	1.00	40.43
C ATOM O	1248	0	GLY	A	282	54.044	36.689	34.184	1.00	39.10
ATOM	1249	· <b>N</b>	ASP	A	283	55.163	35.432	35.671	1.00	40.95
N ATOM	1250	CA	ASP	A	283	56.466	35.918	35.236	1.00	42.89
C ATOM	1251	С	ASP	A	283	57.110	35.037	34.163	1.00	42.30
C ATOM O	1252	0	ASP	Α	283	58.304	35.149	33.903	1.00	43.50
MOTA	1253	CB	ASP	Α	283	57.407	36.046	36.440	1.00	44.35
C ATOM	1254	CG	ASF	A	283	56.985	37.154	37.400	1.00	47.46
C ATOM O	1255	OD1	. ASF	<b>.</b> A	. 283	57.019	38.341	37.000	1.00	47.96
ATOM O	1256	OD2	ASF	) <u>A</u>	283	56.620	36.840	38.555	1.00	48.36

MOTA N	1257	N	LYS	A	284	56.321	34.171	33.534	1.00	42.27
ATOM C	1258	CA	LYS	A	284	56.843	33.283	32.494	1.00	41.83
ATOM C	1259	C	LYS	Α	284	56.953	33.968	31.134	1.00	40.43
ATOM O	1260	0	LYS	A	284	57.689	33.518	30.256	1.00	40.67
ATOM C	1261	CB	LYS	A	284	55.970	32.029	32.360		44.31
ATOM C	1262	CG	LYS	Α	284	56.142	31.005	33.480	1.00	47.22
ATOM C	1263	CD	LYS	A	284	55.534	31.467	34.794	1.00	49.17
ATOM C	1264	CE	LYS	A	284	55.602	30.352	35.837	1.00	51.28
ATOM	1265	NZ	LYS	A	284	54.892	30.695	37.108	1.00	52.23
N ATOM N	1266	N	VAL	A	285	56.204	35.045	30.950	1.00	37.55
ATOM C	1267	CA	VAL	A	285	56. 257	35.784	29.696	1.00	34.84
ATOM C	1268	С.	VAL	A	285	56.954	37.100	30.007	1.00	32.72
ATOM O	1269	0	VAL	A	285	56.514	37.847	30.876	1.00	32.13
ATOM C	1270	СВ	VAL	Α	285	54.846	36.045	29.142	1.00	34.53
ATOM C	1271	CG1	VAL	A	285	54.912	37.015	27.967	1.00	34.19
MOTA	1272	CG2	VAL	A	285	54.224	34.722	28.698	1.00	35.84
C ATOM N	1273	N	LYS	A	286	58.053	37.364	29.307	1.00	31.33
ATOM C	1274	CA	LYS	A	286	58.836	38.575	29.529	1.00	29.68
ATOM C	1275	С	LYS	A	286	58.365	39.710	28.629	1.00	28.86
ATOM O	1276	0	LYS	A	286	58.122	39.509	27.442	1.00	29.10
ATOM .	1277	СВ	LYS	A	.286	•	38.281	29.276	1.00	30.15
ATOM C	1278	CG	LYS	A	286	60.847	37.084	30.062	1.00	29.04
ATOM C	1279	CD	LYS	A	286	60.622	37.263	31.558	1.00	28.26
ATOM C	1280	CE	LYS	A	286	61.158	36.077	32.355	1.00	29.94
ATOM N	1281	NZ	LYS	A	286	60.950	36.259	33.822	1.00	28.63
ATOM N	1282	N	VAL	A	287	58.254	40.907	29.195	1.00	28.83
ATOM C	1283	CA	VAL	Α	287	57.786	42.050	28.427	1.00	28.30
ATOM C	1284	С	VAL	A	287	58.482	43.361	28.793	1.00	27.68

ATOM O	1285	0	VAL	A	287	58.459	43.792	29.942	1.00	28.41
ATOM C	1286	CB	VAL	A	287	56.242	42.211	28.584	1.00	
ATOM	1287	CG1	VAL	A	287	55.874	42.312	30.049	1.00	29.20
C ATOM	1288	CG2	VAL	A	287	55.754	43.436	27.827	1.00	28.74
MOTA N	1289	N	GLY	A	288 .	59.121	43.974	27.803		28.04
ATOM C	1290	CA	GLY	A	288	59.786	45.246	28.025	1.00	26.66
ATOM C	1291	С	GLY	A	288	58.762	46.345	27.815	1.00	26.11
ATOM O	1292	0	GLY	A	288 .	57.721	46.105	27.203	1.00	25.68
ATOM N	1293	N	ALA	A	289	59.044	47.541	28.323	1.00	25.08
ATOM C	1294	CA	ALA	A	289	58.126	48.669	28.192	1.00	24.74
ATOM C	1295	С	ALA	A	289	58.906	49.955	27.935		25.55
MOTA	1296	0	ALA	A	289	60.115	50.007	28.151	1.00	26.30
O ATOM C	1297	СВ	ALA	A	289	57.288	48.813	29.460	1.00	22.88
ATOM N	1298	N	GLY	A	290	58.207	50.990	27.478	1.00	26.17
ATOM C	1299	CA	GLY	A	290	58.857	52.259	27.196	1.00	25.73
ATOM	1300	С	GLY	A	290	58.137	52.974	26.069	1.00	26.32
C ATOM O	1301	0	GLY	A	290	57.099	52.500	25.616	1.00	27.48
ATOM N	1302	N	ASN	A	291	58.677	54.095	25.592	1.00	25.49
MOTA	1303	CA	ASN	A	291	59.932	54.659	26.,086	1.00	24.28
C ATOM	1304	С	ASN	A	291	59.744	55.754	27.124	1.00	23.86
C ATOM	1305	0	ASN	Α	291	58.738	56.465	27.115	1.00	22.00
O ATOM	1306	СВ	ASN	Α	291	60.729	55.245	24.919	1.00	24.80
C ATOM C	1307	CG	ASN	Α	291	61.287	54.184	24.008	1.00	25.31
ATOM O	1308	OD1	ASN	Α	291	60.830	53.042	24.021	1.00	25.35
ATOM N	1309	ND2	ASN	Α	291	62.278	54.555	23.202	1.00	24.45
ATOM N	1310	N	ILE	A	. 292	60.729	55.883	28.011	1.00	22.96
ATOM C	1311	CA	ILE	A	. 292	60.724	56.925	29.030	1.00	22.95
ATOM C	1312	С	ILE	A	292	62.077	57.636	28.986	1.00	23.91

ATOM O	1313	0	ILE	A	292	63.017	57.157	28.342	1.00	23.07
ATOM C	1314	СВ	ILE	A	292	60.426	56.356	30.455	1.00	23.66
MOTA	1315	CG1	ILE	A	292	61.301	55.139	30.770	1.00	22.82
C ATOM C	1316	CG2	ILE	A	292	58.958	55.963	30.542	1.00	24.06
ATOM C	1317	CD1	ILE	A	292	62.734	55.478	31.158	1.00	23.86
ATOM	1318	N	VAL	A	293	62.181	58.791	29.633	1.00	24.59
N ATOM C	1319	CA	VAL	A	293	63.440	59.524	29.605	1.00	25.09
ATOM C	1320	С	VAL	A	293	63.902	60.057	30.944	1.00	25.38
MOTA	1321	0	VAL	A	293	64.874	60.812	31.000	1.00	24.51
O ATOM C	1322	СВ	VAL	A	293	63.380	60.708	.28.623	1.00	24.93
ATOM C	1323	CG1	VAL	A	293	63.283	60.192	27.196	1.00	24.14
ATOM	1324	CG2	VAL	A	293	62.200	61.601	28.965	1.00	25.29
N ATOM C	1325	N	ASP	A	294	63.209	59.686	32.018	1.00	25.36
ATOM C	1326	CA	ASP	Α	294	63.610	60.140	33.342	1.00	25.43
ATOM	1327	С	ASP	A	294	63.315	59.123	34.439	1.00	25.22
C ATOM O	1328	.0	ASP	A	294	62.705	58.082	34.188	1.00	24.53
ATOM C	1329	СВ	ASP	A	294	62.966	61.500	33.678	1.00	26.32
ATOM C	1330	CG	ASP	Α	294	61.456	61.424	33.890	1.00	26.90
ATOM O	1331	OD1	ASP	A	294	60.831	60.369	33.659	1.00	27.35
ATOM O	1332	OD2	ASP	A	294	60.884	62.456	34.291	1.00	28.46
MOTA	1333	N	GLY	A	295	63.762	59.435	35.649	1.00	25.01
N ATOM C	1334	CA	GLY	A	295	63.561	58.540	36.774	1.00	26.69
ATOM C	1335	С	GLY	A	295	62.112	58.224	37.083	1.00	26.45
ATOM O	1336	0	GLY	A	295	61.778	57.086	37.408	1.00	25.94
ATOM	1337	N	GLU	A	296	61.243	59.225	36.991	1.00	27.48
N ATOM C	1338	CA	GLU	A	296	59.825	59.013	37.275	1.00	27.87
ATOM C	1339	С	GLU	A	296	59.191	58.014	36.317	1.00	27.05
ATOM O	1340	0	GLU	A	296	58.438	57.136	36.736	1.00	26.56
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ATOM C	1341	СВ	GLU	A	296	59.066	60.340	37.211	1.00	31.37
ATOM C	1342	CG	GLU	A	296	59.445	61.302	38.318	1.00	37.66
ATOM C	1343	CD	GLU	A	296	58.542	62.513	38.368	1.00	42.29
ATOM O	1344	OE1	GLU	A	296	57.320	62.336	38.576	1.00	45.55
ATOM O	1345	OE2	GLU	Α	296	59.050	63.643	38.196		45.27
ATOM N	1346	N	GLY	A	297	59.492	58.155	35.030	1.00	25.33
ATOM C	1347	CA	GLY	Α	297	58.939	57.249	34.042	1.00	25.17
ATOM C	1348	С	GLY	Α	297	59.456	55.839	34.273	1.00	25.62
MOTA O	1349	0	GLY	A	297	58.719	54.863	34.137	1.00	24.83
	1350	N	PHE	A	298	60.737	55.734	34.610	1.00	24.52
ATOM C	1351 .	CA	PHE	Α	298	61.343	54.434	34.880		25.70
ATOM C	1352	С	PHE	A	298	60.631	53.751	36.043	1.00	26.22
ATOM O	1353	0	PHE	A	298	60.219	52.595	35.946	1.00	26.55
ATOM C	1354	CB	PHE	A	298	62.821	54.589	35.253	1.00	24.99
ATOM C	1355	CG	PHE	A	298	63.432	53.322	35.785	1.00	24.97
ATOM C	1356	CD1	PHE	A	298	63.935	52.358	34.917	1.00	25.29
ATOM C	1357	CD2	PHE	A	298	63.410	53.047	37.150	1.00	25.62
ATOM C	1358	CE1	PHE	A	298	64.400	51.131	35.400	1.00	25.51
ATOM C	1359	CE2	PHE	A	298	63.871	51.822	37645	1.00	25.63
ATOM C	1360	CZ	PHE	A	298	64.364	50.863	36.766	1.00	23.87
ATOM N	1361	N	ARG	A	299	60.504	54.478	37.149	1.00	26.18
ATOM C	1362	CA	ARG	A	299	59.875	53.947	38.354	1.00	27.35
ATOM C	1363	С	ARG	A	299	58.440	53.489	38.104	1.00	27.07
ATOM O	1364	0	ARG	A	299	58.011	52.454	38.622	1.00	26.36
ATOM C	1365	CB	ARG	A	299	59.916	55.000	39.468	1.00	28.99
ATOM C	1366	CG	ARG	A	299	59.457	54.503	40.837	1.00	32.84
ATOM C	1367	CD	ARG	A	299	59.794	55.518	41.926	1.00	35.60
ATOM N	1368	NE	ARG	A	299	61.220	55.543	42.252	1.00	37.71

ATOM C	1369	CZ	ARG	A	299	61.834	54.631	43.006	1.00	38.54
ATOM N	1370	NH1	ARG	A	299	61.150	53.616	43.519	1.00	37.82
ATOM N	1371	NH2	ARG	A	299	63.133	54.738	43.258	1.00	38.76
ATOM N	1372	N	TYR	A	300	57.702	54.249	37.303	1.00	25.60
ATOM C	1373	CA	TYR	A	300	56.324	53.890	37.005	1.00	25.92
ATOM C	1374	С	TYR	A	300	56.249	52.543	36.286	1.00	26.46
ATOM O	1375	0	TYR	A	300	55.431	51.690	36.634	1.00	26.22
ATOM C	1376	CB	TYR	A	300	55.664	54.958	36.136	1.00	26.45
ATOM C	1377	CG	TYR	A	300	54.209	54.667	35.845	1.00	26.38
ATOM C	1378	CD1	TYR	Α	300	53.222	54.911	36.803	1.00	27.42
ATOM C	1379	CD2	TYR	Α	300	53.822	54.123	34.623	1.00	26.65
ATOM C	1380	CE1	TYR	A	300	51.881	54.621	36.546	1.00	27.66
ATOM C	1381	CE2	TYR	A	300	52.486	53.831	34.359	1.00	26.96
ATOM C	1382	CZ	TYR	A	300	51.525	54.083	35.321	1.00	27.35
ATOM O	1383	OH	TYR	A	300	50.207	53.804	35.045	1.00	28.84
MOTA	1384	N	LEU	A	301	57.100	52.352	35.283	1.00	24.93
N ATOM C	1385	CA	LEU	A	301	57.097	51.101	34.539	1.00	25.20
ATOM C	1386	С	LEU	A	301	57.727	49.962	35.343	1.00	24.99
ATOM O	1387	0	LEU	A	301	57.383	48.795	35.152	1.00	25.51
ATOM C	1388	СВ	LEU	A	301	57.814	51.281	33.192	1.00	24.73
ATOM C	1389	CG	LEU	A	301	57.092	52.216	32.208	1.00	24.97
ATOM C	1390	CD1	LEU	A	301	57.901	52.348	30.920	1.00	24.19
ATOM C	1391	CD2	LEU	A	301	55.693	51.665	31.903	1.00	25.94
MOTA N	1392	N	ALA	A	302	58.642	50.300	36.243	1.00	25.01
	1393	CA	ALA	A	302	59.284	49.289	37.077	1.00	26.34
ATOM C	1394	С	ALA	A	302	58.224	48.715	38.022	1.00	27.09
ATOM O	1395	0	ALA	A	302	58.068	47.495	38.140	1.00	27.29
ATOM C	1396	CB	ALA	A	302	60.426	49.911	37.872	1.00	25.08

ATOM N	1397	N	ASP	A	303	57.493	49.603	38.688	1.00	27.62
ATOM C	1398	CA	ASP	A	303	56.439	49.182	39.602	1.00	29.54
ATOM C	1399	С	ASP	A	303	55.335	48.444	38.853	1.00	29.82
ATOM O	1400	0	ASP	A	303	54.670	47.574	39.423	1.00	29.45
ATOM C	1401	CB	ASP	A	303	55.846	50.386	40.342	1.00	31.26
ATOM C	1402	CG	ASP	A	303	56.796	50.967	41.374	1.00	34.06
ATOM O	1403	OD1	ASP	A	303	57.678	50.226	41.863	1.00	35.03
ATOM O	1404	OD2	ASP	A	303	56.652	52.160	41.713	1.00	35.59
ATOM N	1405	N	ALA	A	304	55.145	48.786	37.579	1.00	28.20
ATOM C	1406	CA	ALA	A	304	54.124	48.148	36.748	1.00	28.48
ATOM C	1407	C	ALA	A.	304	54.500	46.706	36.403	1.00	29.41
ATOM O	1408	. О	AĻA	A	304	53.644	45.919	35.981	1.00	30.01
ATOM C	1409	СВ	ALA	A	304	53.913	48.943	35.467	1.00	29.13
ATOM N	1410	N	GLY	A	305	55.779	46.371	36.558	1.00	27.94
ATOM C	1411	CA	GLY	A	305	56.228	45.013	36.285	1.00	28.09
ATOM C	1412	C	GLY	A	305	57.047	44.759	35.031	1.00	27.94
ATOM O	1413	0	GLY.	Α	305	57.303	43.603	34.688	1.00	28.94
ATOM N	1414	N	ALA	A	306	57.468	45.815	34.342	1.00	27.01
ATOM C	1415	CA	ALA	A	306	58.259	45.655	33.118	1.00	26.21
ATOM C	1416	C	ALA	A	306	59.530	44.833	33.371	1.00	25.71
ATOM O	1417	Ο,-	ALA	A	306	60.172	44.983	34.409	1.00	26.47
ATOM C	1418	CB	ALA	A	306	58.630	47.038	32.549	1.00	26.19
ATOM N	1419	N	ASP	A	307	59.888	43.970	32.421	1.00	26.45
ATOM C	1420	CA	ASP	A	307	61.087	43.135	32.549	1.00	26:38
ATOM C	1421	С	ASP	A	307	62.351	43.883	32.137	1.00	26.11
ATOM O	1422	0	ASP	A	307	63.459	43.517	32.523	1.00	26.90
ATOM C	1423	CB	ASP	A	307	60.923	41.857	31.731	1.00	27.11
ATOM C	1424	CG	ASP	A	307	59.967	40.887	32.387	1.00	29.35

ATOM O	1425	OD1	ASP	A	307	60.312	40.373	33.470	1.00	29.58
ATOM O	1426	OD2	ASP	A	307	58.873	40.656	31.837	1.00	30.28
ATOM N	1427	N	PHE	A	308	62.174	44.916	31.324	1.00	24.79
ATOM C	1428	CA	PHE	A	308	63.274	45.786	30.922	1.00	25.02
ATOM C	1429	С	PHE	A	308	62.613	47.071	30.453	1.00	25.26
ATOM O	1430	Ο,	PHE	A	308	61.465	47.059	30.006	1.00	25.39
ATOM C	1431	СВ	PHE	A	308	64.194	45.142	29.855	1.00	24.16
ATOM C	1432	CG	PHE	A	308	63.647	45.131	28.449	1.00	26.91
ATOM C	1433	CD1	PHE	A	308	63.601	46.297	27.686	1.00	26.51
ATOM C	1434	CD2	PHE	A	308	63.232	43.933	27.866	1.00	27.59
ATOM C	1435	CE1	PHE	A	308	63.157	46.273	26.368	1.00	27.45
ATOM C	1436	CE2	PHE	A	308	62.783	43.892	26.543	1.00	28.40
ATOM C	1437	CZ	PHE	A	308	62.745	45.062	25.790	1.00	28.01
ATOM N	1438	N	ILE	Α	309	63.316	48.187	30.597	1.00	24.66
ATOM C	1439	CA	ILE	A	309	62.737	49.469	30.227	1.00	24.56
ATOM C	1440	C	ILE	Α	309	63.565	50.185	29.171	1.00	24.22
ATOM O	1441	.0	ILE	A	309	64.781	50.319	29.304	1.00	23.11
ATOM C	1442	CB	ILE	A	309	62.566	50.338	31.495	1.00	25.23
ATOM C	1443	CG1	ILE	Α	309	61.544	49.662	32.419	1.00	24.51
ATOM C	1444	CG2	ILE	A	309	62.134	51.756	31.123	1.00	24.72
ATOM C	1445	CD1	ILE	A	309	61.450	50.243	33.802	1.00	25.49
ATOM N	1446	N	LYS	A	310	62.881	50.643	28.125	1.00	23.39
ATOM C	1447	CA	LYS	Α	310	63.527	51.310	27.003	1.00	24.09
ATOM C	1448	С	LYS	A	310	63.573	52.825	27.202	1.00	24.12
MOTA O	1449	0	LYS	A	310	62.578	53.449	27.575	1.00	22.87
ATOM C	1450	CB	LYS	A	310	62.788	50.945	25.713	1.00	25.57
ATOM C	1451	CG	LYS	A	310	63.633	51.022	24.457	1.00	27.69
ATOM C	1452	CD	LYS	Α	310	63.347	49.838	23.526	1.00	27.60

ATOM C	1453	CE	LYS	A	310	61.915	49.849	23.020	1.00	27.87
ATOM N	1454	NZ	LYS	A	310	61.614	51.110	22.280	1.00	28.37
ATOM N	1455	N	ILE	A	311	64.741	53.398	26.925	1.00	23.23
ATOM C	1456	CA	ILE	A	311	64.996	54.827	27.101	1.00	23.17
ATOM C	1457	С	ILE	A	311	65.173	55.586	25.794	1.00	21.87
ATOM O	1458	0	ILE	A	311	65.937	55.166	24.925	1.00	22.46
ATOM C	1459	CB	ILE	A	311	66.301	55.045	27.901	1.00	21.23
ATOM C	1460	CG1	ILE	A	311	66.238	54.291	29.236	1.00	22.02
ATOM C	1461	CG2	ILE	A	311	66.537	56.532	28.122	1.00	21.42
ATOM C	1462	CD1	ILE	A	311	67.601	54.143	29.891	1.00	21.94
ATOM N	1463	N	GLY	A	312	64.484	56.712	25.662	1.00	24.32
ATOM C	1464	CA	GLY	Α	312	64.666	57.510	24.467	1.00	24.57
ATOM C	1465	С	GLY	A	312	63.449	58.070	23.773	1.00	26.09
MOTA O	1466	0	GLY	Α	312	62.559	57.332	23.356	1.00	25.55
ATOM N	1467	N	ILE	Α.	313	63.428	59.393	23.644	1.00	26.99
ATOM C	1468	CA	ILE	A	313	62.357	60.089	22.950	1.00	28.73
ATOM C	1469	С	ILE	A	313	62.968	61.275	22.215	1.00	30.51
ATOM O	1470	0	ILE	A	313	63.531	62.172	22.845	1.00	30.13
ATOM C	1471	CB	ILE	A	313	61.281	60.635	23.915	1.00	28.78
ATOM C	1472	CG1	ILE	Α	313	60.561	59.480	24.619	1.00	29.45
ATOM C	1473	CG2	ILE	A	313	60.277	61.469	23.13.4	1.00	29.20
ATOM C	1474	CD1	ILE	A	313	59.544	59.942	25.648	1.00	29.69
MOTA N	1475	N	GLY	A	314	62.865	61.264	20.888	1.00	33.20
ATOM C	1476	CA	GLY	A	314	63.385	62.357	20.087	1.00	36.88
ATOM C	1477	С	GLY	A	314	64.748	62.144	19.454	1.00	39.48
MOTA O	1478	0	GLY	A	314	65.102	62.843	18.499	1.00	40.62
ATOM N	1479	N	GLY	A	315	65.506	61.177	19.967	1.00	40.05
ATOM C	1480	CA	GLY	A	315	66.840	60.918	19.452	1.00	41.12

ATOM C	1481	С	GLY	A	315	66.950	60.152	18.146	1.00	42.12
ATOM O	1482	0	GLY	A	315	67.977	60.235	17.469	1.00	41.49
ATOM N	1483	N	GLY	A	316	65.906	59.409	17.790	1.00	42.04
ATOM C	1484	CA	GLY	A	316	65.924	58.640	16.555	1.00	42.81
ATOM C	1485	С	GLY	A	316	66.345	59.447	15.338	1.00	43.59
ATOM O	1486	0	GLY	A	316	66.029	60.633	15.227	1.00	44.04
ATOM N	1487	N	SER	A,	317	67.056	58.800	14.419	1.00	44.63
ATOM C	1488	CA	SER	A	317	67.535 ,	59.453	13.204	1.00	45.96
ATOM C	1489	С	SER	A	317	66.400	59.929	12.303	1.00	47.12
ATOM O	1490	0	SER	A	317	66.554	60.897.	11.561	1.00	46.76
ATOM C	1491	CB	SER	Α	317	68.436	58.503	12.412	1.00	45.33
ATOM O	1492	OG	SER	A	317	67.704	57.391	11.925	1.00	44.82
ATOM N	1493	N	ILE	A	318	65.266	59.240	12.363	1.00	49.21
ATOM C	1494	CA	ILE	A	318	64.115	59.604	11.544	1.00	51.92
ATOM C	1495	С	ILE	A	318	62.986	60.204	12.374	1.00	53.83
ATOM O	1496	0	ILE	A	318	61.811	60.095	12.019	1.00	54.17
ATOM C	1497	CB	ILE	A	318	63.581	58.381	10.754	1.00	51.77
ATOM C	1498	CG1	ILE	A	318	63.731	57.105	11.586	1.00	51.59
ATOM C	1499	CG2	ILE	A	318	64.339	58.237	9.441	1.00	51.61
ATOM C	1500	CD1	ILE	A	318	62.997	57.131	12.898	1.00	51.22
HETATM N	1501	N	cso	A	319	63.355	60.840	13.481	1.00	56.01
HETATM C	1502	CA	CSO	A	319	62.387	61.468	14.371	1.00	58.61
HETATM C	1503	СВ	CSO	A	319	62.457	60.825	15.760	1.00	60.16
HETATM S	1504	SG	cso	A	319	60.983	61.106	16.793	1.00	64.08
HETATM C	1505	С	cso	A	319	62.708	62.957	14.481	1.00	59.03
HETATM O	1506	0	cso	A	319	63.754	63.331	15.008	1.00	58.88
HETATM O	1507	OD	CSO	A	319	60.477	62.837	16.987	1.00	63.19
ATOM N	1508	N	ILE	A	320	61.814	63.805	13.979	1.00	59.78

ATOM	1509	CA	ILE	Α	320	62.028	65.250	14.034	1.00	60.48
C	•									
ATOM C	1510	С	ILE	A	320	61.159	65.875	15.125	1.00	60.65
ATOM O	1511	0	ILE	A	320	60.074	66.397	14.856	1.00	60.82
ATOM C	1512	СВ	ILE	A	320	61.706	65.913	12.676	1.00	60.96
ATOM C	1513	CG1	ILE	A	320	62.500	65.221	11.562	1.00	61.17
ATOM C	1514	CG2	ILE	Α	320	62.064	67.398	12.721	1.00	60.93
ATOM C	1515	CD1	ILE	A	320	62.196	65.738	10.167	1.00	61.13
ATOM N	1516	N	THR	A	321	61.656	65.817	16.357	1.00	60.47
ATOM C	1517	CA	THR	A	321	60.961	66.343	17.530	1.00	60.58
ATOM C	1518	C	THR	A	321	60.288	67.701	17.323	1.00	60.31
ATOM	1519	0	THR	A	321	59.072	67.828	17.474	1.00	59.52
ATOM C	1520	СВ	THR	Α	321	61.928	66.469	18.726	1.00	60.88
ATOM O	1521	OG1	THR	A	321	62.632	65.234	18.906	1.00	61.19
ATOM C	1522	CG2	THR	A	321	61.157	66.797	19.995	1.00	60.45
ATOM N	1523	N	ARG	A	322	61.086	68.709	16.986	1.00	60.45
ATOM C	1524	CA	ARG	A	322	60.581	70.063	16.776	1.00	60.85
MOTA	1525	С	ARG	A	322	59.375	70.172	15.850	1.00	60.80
C ATOM O	1526	0	ARG	Α	322	58.401	70.849	16.176	1.00	60.73
ATOM C	1527	CB	ARG	A	322	61.695	70.967	16.251	1.00	61.37
MOTA	1528	CG	ARG	A	322	62.696	71.397	17.305	1.00	62.07
C ATOM	1529	CD	ARG	A	322	63.711	72.351	16.706	1.00	62.95
C ATOM	1530	NE	ARG	A	322	64.504	73.029	17.726	1.00	63.47
N ATOM C	1531	CZ	ARG	A	322	65.442	73.931	17.458	1.00	63.65
ATOM N	1532	NH1	ARG	A	322	65.704	74.262	16.200	1.00	63.49
ATOM N	1533	NH2	ARG	A	322	66.115	74.504	18.445	1.00	63.65
ATOM N	1534	N	GLU	A	323	59.437	69.522	14.693	1.00	60.59
ATOM C	1535	CA	GLU	A	323	58.328	69.579	13.747	1.00	60.45
ATOM C	1536	С	GLU	A	323	57.157	68.717	14.208	1.00	59.48

ATOM O	1537	0	GLU	A	323	56.231	68.454	13.439	1.00	59.76
ATOM C	1538	CB	GLU	A	323	58.781	69.116	12.359	1.00	61.67
ATOM	1539.	CG	GLU	A	323	59.935	69.914	11.778	1.00	63.67
ATOM C	1540	CD	GLU	A	323	60.259	69.515	10.348	1.00	64.69
ATOM O	1541	OE1	GLU	Α	323	60.474	68.311	10.094	1.00	65.62
ATOM O	1542	OE2	GLU	A	323	60.301	70.407	9.476	1.00	65.47
ATOM N	1543	N	GLN	A	324	57.194	68.284	15.464	1.00	57.92
ATOM C	1544	CA	GLN	A	324	56.131	67.446	16.001	1.00	56.25
ATOM C	1545	С	GLN	A	324	55.529	67.984	17.300	1.00	54.10
ATOM O	1546	0	GLN	A	324	54.872	69.026	17.300	1.00	54.39
ATOM C	1547	СВ	GLN	Α	324	56.653	66.022	16.206	1.00	58.06
ATOM C	1548	CG	GLN	Α	324	57.155	65.370	14.924	1.00	60.13
ATOM C	1549	CD	GLN	A	324	57.820	64.027	15.164	1.00	61.81
ATOM O	1550	OE1	GLN	A	324	58.311	63.388	14.231	1.00	62.58
ATOM N	1551	NE2	GLN	A	324	57.838	63.590	16.419	1.00	62.80
ATOM N	1552	N	LYS	A	325	55.754	67.278	18.404	1.00	50.55
ATOM C	1553	CA	LYS	A	325	55.200	67.685	19.693	1.00	46.97
ATOM C	1554	С	LYS	A	325	56.157	68.456	20.589	1.00	43.59
ATOM O	1555	0	LYS	Α,	325	55.731	69.086	21.558	1.00	42.57
ATOM C	1556	СВ	LYS	A	325	54.703	66.463	20.467	1.00	47.99
ATOM -	1557	CG	LYS	A	325	53.491	65.775	19.876	1.00	50.14
ATOM C	1558	CD	LYS	A	325	53.077	64.618	20.773	1.00	50.62
ATOM C	1559	CE	LYS	A	325	51.895	63.874	20.208	1.00	51.86
ATOM N	1560	NZ	LYS	A	325	51.526	62.721	21.067	1.00	52.95
ATOM N	1561	N	GLY	Α	326	57.446	68.400	20.283	1.00	39.82
ATOM C	1562	CA	GLY	A	326	58.399	69.103	21.118	1.00	36.97
ATOM C	1563	C	GLY	Α	326	58.613	68.383	22.439	1.00	35.12
ATOM O	1564	0	GLY	A	326	58.842	69.015	23.473	1.00	33.70

ATOM N	1565	N	ILE	A	327	58.510	67.056	22.412	1.00	33.10
ATOM C	1566	CA	ILE	A	327	58.732	66.255	23.609	1.00	31.94
ATOM C	1567	С	ILE	A	327	60.039	65.500	23.399	1.00	30.96
ATOM O	1568	0	ILE	A	327	60.360	65.095	22.283	1.00	29.97
ATOM C	1569	CB	ILE	A	327	57.584	65.229	23.865	1.00	33.54
ATOM C	1570	CG1	ILE	A	327	57.479	64.236	22.708	1.00	35.09
ATOM C	1571	CG2	ILE	A	327	56.257	65.961	24.048	1.00	34.89
ATOM C	1572	CD1	ILE	A	327	56.438	63.139	22.937	1.00	37.76
ATOM N	1573	N	GLY	A	328	60.807	65.322	24.463	1.00	29.65
ATOM C	1574	CA	GLY	A	328	62.058	64.606	24.312	1.00	29.68
ATOM C	1575	С	GLY	A.	328	63.106	65.030	25.316	1.00	28.25
ATOM O	1576	0	GLY	A	328	62.838	65.825	26.220	1.00	27.09
ATOM N	1577	N	ARG	A	329	64.309	64.494	25.147	1.00	27.34
ATOM C	1578	CA	ARG	A	329	65.410	64.807	26.039	1.00	26.13
ATOM C	1579	С	ARG	A	329	66.674	64.258	25.404	1.00	25.89
ATOM O	1580	0	ARG	A	329	66.636	63.207	24.760	1.00	25.64
ATOM C	1581	CB	ARG	À	329	65.178	64.141	27.400	1.00	26.27
ATOM C	1582	CG	ARG	A	329	66.074	64.661	28.510	1.00	25.63
ATOM C	1583	CD	ARG	Α	329	65.816	63.929	29.809	1.00	25.44
ATOM N	1584	NE	ARG	A	329	66.249	64.709	30.966	1.00	24.87
ATOM C	1585	CZ	ARG	A	329	66.203	64.269	32.218	1.00	26.41
ATOM N	1586	NH1	ARG	A	329	65.754	63.048	32.475	1.00	25.65
NOTA	1587	NH2	ARG	A	329	66.577	65.058	33.216	1.00	26.64
ATOM N	1588	N	GLY	A	330	67.787	64.975	25.560	1.00	25.19
ATOM C	1589	CA	GLY	A	330	69.040	64.497	25.002	1.00	24.58
ATOM C	1590	С	GLY	A	330	69.218	63.063	25.469	1.00	24.73
ATOM O	1591	0	GLY	Α	330	69.010	62.770	26.645	1.00	23.16
ATOM N	1592	N	GLN	A	331	69.617	62.174	24.566	1.00	24.37

ATOM C	1593	CA	GĽŅ	A	331	69.763	60.757	24.909	1.00	24.78
ATOM C	1594	С	GLN	Α	331	70.739	60.463	26.043	1.00	24.31
ATOM O	1595	0	GLN	A	331	70.466	59.610	26.889	1.00	23.63
ATOM C	1596	СВ	GLN	A	331	70.162	59.947	23.667	1.00	25.13
ATOM C	1597	CG	GLN	A	331	70.073	58.430	23.863	1.00	25.46
ATOM C	1598	CD	GLN	Α	331	68.633	57.917	23.958		28.00
ATOM O	1599	OE1	GLN	A	331	68.391	56.774	24.355	1.00	29.62
ATOM N	1600	NE2	GLN	A	331	67.679	58.756	23.586	1.00	26.29
ATOM N	1601	N	ALA	A	332	71.878	61.155	26.064	1.00	23.62
ATOM C	1602	CA	ALA	A	332	72.864	60.930	27.117	1.00	22.91
ATOM C	1603	С	ALA	A	332	72.283	61.243	28.492	1.00	23.37
ATOM O	1604	0	ALA	Α	332	72.389	60.441	29.425	1.00	22.61
ATOM C	1605	СВ	ALA	A	332	74.115	61.778	26.864	1.00	23.28
ATOM N	1606	N	THR	A	333	71.668	62.413	28.619	1.00	22.11
ATOM C	1607	CA	THR	A	333	71.075	62.815	29.878	1.00	22.48
ATOM C	1608	C	THR	A	333	69.974	61.840	30.296	1.00	22.58
ATOM O	1609	0	THR	A	333	69.857	61.492	31.470	1.00	21.18
ATOM C	1610	CB	THR	A	333	70.493	64.238	29.785	1.00	23.93
ATOM O	1611	ÓG1	THR	A	333	71.547	65.160	29.457	1.00	24.95
ATOM C	1612	CG2	THR	A	333	69.865	64.645	31.119	1.00	23.81
ATOM N	1613	N	ALA	A	334	69.176	61.401	29.329	1.00	21.99
ATOM C	1614	CA	ALA	A	334	68.093	60.462	29.600	1.00	22.69
ATOM C	1615	С	ALA	A	334	68.630	59.149	30.178	1.00	22.31
ATOM O	1616	0	ALA	A	334	68.113	58.632	31.175	1.00	22.17
ATOM C	1617	CB	ALA	A	334	67.315	60.186	28.319	1.00	22.40
ATOM N	1618	N	VAL	A	335	69.663	58.604	29.548	1.00	22.74
ATOM C	1619	CA	· VAL	A	335	70.248	57.349	30.019	1.00	21.65
ATOM C	1620	С	VAL	A	335	70.836	57.522	31.417	1.00	22.93

ATOM O	1621	0	VAL	A	335	70.561	56.739	32.327	1.00	22.43
ATOM C	1622	СВ	VAL	Α	335	71.360	56.864	29.062	1.00	23.64
ATOM C	1623	CG1	VAL	A	335	72.090	55.646	29.664	1.00	22.43
ATOM C	1624	CG2	VAL	A	335	70.750	56.502	27.712	1.00	22.06
MOTA N	1625	N	ILE	A	336	71.644	58.562	31.590	1.00	22.47
ATOM C	1626	CA	ILE	Α	336	72.275	58.816	32.879	1.00	22.53
ATOM C	1627	C	ILE	A	336	71.251	58.936	34.005	1.00	23.00
ATOM O	1628	0	ILE	A	336	71.418	58.363	35.087	1.00	21.54
ATOM C	1629	CB	ILE	A	336	73.132	60.097	32.810	1.00	22.52
ATOM C	1630	CG1	ILE	A	336	74.304	59.869	31.846	1.00	21.96
ATOM .	1631	CG2	ILE	A	336	73.639	60.476	34.199	1.00	23.53
ATOM C	1632	CD1	ILE	Α	336	75.114	61.125.	31.544	1.00	24.57
ATOM N	1633	N	ASP	A	337	70.183	59.679	33.745	1.00	23.52
ATOM C	1634	CA	ASP	A	337	69.146	59.880	34.750	1.00	23.90
ATOM C	1635	С	ASP	A	337	68.406	58.575	35.066	1.00	23.59
ATOM O	1636	0	ASP	A	337	68.220	58.212	36.234	1.00	22.64
ATOM C	1637	CB	ASP	A	337	68.153	60.931	34.251	1.00	26.45
ATOM C	1638	CG	ASP	A	337	67.150	61.326	35.301	1.00	28.83
ATOM O	1639	OD1	ASP	A	337	65.975	61.536	34.943	1.00	30.37
ATOM O	1640	OD2	ASP	A	337	67.539	61.437	36.483	1.00	32.41
ATOM N	1641	N	VAL	A	338	67.982	57.870	34.024	1.00	22.38
ATOM C	1642	CA	VAL	A	338	67.258	56.619	34.221	1.00	23.04
ATOM C	1643	C ,	VAL	A	338	68.116	55.587	34.949	1.00	23.56
ATOM O	1644	0	VAL	A	338	67.635	54.899	35.852	1.00	23.29
ATOM C	1645	СВ	VAL	A	338	66.776	56.030	32.875	1.00	22.58
ATOM C	1646	CG1	VAL	A	338	66.198	54.625	33.089	1.00	21.84
ATOM C	1647	CG2	VAL	A	338	65.707	56.941	32.269	1.00	21.24
ATOM N	1648	N	VAL	A	339	69.383	55.489	34.559	1.00	23.76

ATOM C	1649	CA	LAV	A	339	70.292	54.542	35.189	1.00	23.00
ATOM C	1650	С	VAL	A	339	70.446	54.832	36.682	1.00	24.41
MOTA	1651	0	VAL	A	339	70.499	53.906	37.496	1.00	23.06
O ATOM C	1652	CB	VAL	A	339	71.677	54.563	34.497	1.00	23.80
ATOM C	1653	CG1	VAL	A	339	72.729	53.905	35.382	1.00	22.59
ATOM C	1654	CG2	VAL	Α	339	71.588	53.822	33.164	1.00	22.47
ATOM N	1655	N	ALA	A	340	70.512	56.110	37.045	1.00	23.21
ATOM C	1656	CA	ALA	A	340	70.644	56.478	38.452	1.00	24.61
ATOM C	1657	С	ALA	A	340	69.413	55.992	39.214	1.00	25.25
ATOM O	1658	0	ALA	A	340	69.520	55.462	40.326	1.00	24.89
ATOM C	1659	СВ	ALA	A	340	70.783	57.992	38.591	1.00	25.22
ATOM N	1660	N	GLU	A	341	68.243	56.168	38.608	1.00	24.78
ATOM C	1661	CA	GLU	Α	341	66.995	55.749	39.237	1.00	25.88
ATOM C	1662	С	GLU	A	341	66.917	54.228	39.310	1.00	25.65
ATOM O	1663	0	GLU	Α	341	66.422	53.672	40.291	1.00	25.06
ATOM	1664	CB	GLU	A	341	65.799	56.283	38.449	1.00	26.19
C ATOM C	1665	CG	GLU	A	341	64.465	56.213	39.194	1.00	30.02
	1666	CD	GLU	A	341	64.419	57.128	40.411	1.00	33.39
ATOM O	1667	OE1	GLU	A	341	64.983	58.241	40.350	1.00	35.47
ATOM O	1668	OE2	GLU	Α	341	63.804	56.744	41.424	1.00	35.11
ATOM ·	1669	N	ARG	A	342	67.403	53.566	38.265	1.00	25.58
ATOM C	1670	CA	ARG	A	342	67.399	52.106	38.198	1.00	25.78
ATOM C	1671	С	ARG	A	342	68.295	51.531	39.300	1.00	25.93
ATOM O	1672	0 .	ARG	A	342	67.952	50.528	39.932	1.00	26.38
ATOM C	1673	CB	ARG	A	342	67.878	51.651	36.803	1.00	24.64
ATOM C	1674	CG	ARG	A	342	67.855	50.138	36.546	1.00	24.33
ATOM C	1675	CD	ARG	A	342	69.100	49.431	37.092	1.00	23.54
ATOM N	1676	NE	ARG	A	342	70.350	49.884	36.477	1.00	22.90

ATOM C	1677	CZ	ARG	A	342	70.718	49.640	35.220	1.00	23.00
ATOM N	1678	NH1	ARG	Α	342	69.934	48.943	34.406	1.00	21.73
ATOM N	1679	NH2	ARG	A	342	71.893	50.075	34.778	1.00	23.48
ATOM N	1680	N	ASN	A	343	69.440	52.166	39.534	1.00	25.49
ATOM C	1681	CA	ASN	A	343	70.355	51.697	40.571	1.00	27.07
ATOM C	1682	C	ASN	A	343	69.774	51.944	41.964	1.00	27.92
ATOM O	1683	0	ASN	A	343	69.976	51.150	42.887	1.00	27.27
ATOM C	1684	CB	ASN	A	343	71.722	52.373	40.422	1.00	27.28
ATOM C	1685	CG	ASN	A	343	72.457	51.921	39.171	1.00	28.20
ATOM O	1686	OD1	ASN	Ά	343	72.178	50.844	38.634	1.00	27.39
ATOM N	1687	ND2	ASN	A	343	73.412	52.728	38.712	1.00	27.58
ATOM	1688	N	LYS	A	344	69.042	53.044	42.108	1.00	27.67
N ATOM C	1689	CA	LYS	A	344	68.402	53.376	43.374	1.00	29.76
ATOM C	1690	С	LYS	A	344	67.313	52.334	43.617	1.00	29.60
ATOM O	1691	0	LYS	A	344	67.162	51.810	44.726	1.00	30.86
ATOM C	1692	CB	LYS	A	344	67.790	54.780	43.290	1.00	31.91
ATOM C	1693	CG	LYS	A	344	67.158	55.286	44.574	1.00	37.21
ATOM C	1694	CD	LYS	A	344	66.732	56.745	44.414	1.00	40.26
ATOM C	1695	CE	LYS	A	344	66.241	57.339	45.725	1.00	42.77
ATOM N	1696	NZ	LYS	A	344	66.010	58.812	45.594		44.75
ATOM N	1697	N	TYR	A	345	66.564	52.023	42.564	1.00	28.67
ATOM C	1698	CA	TYR	A	345	65.491	51.034	42.640	1.00	28.68
ATOM C	1699	С	TYR	A	345	66.042	49.669	43.064	1.00	29.72
ATOM O	1700	0	TYR	A	345	65.456	48.977	43.902	1.00	29.46
ATOM C	1701	CB	TYR	A	345	64.816	50.896	41.280	1.00	27.98
ATOM C	1702	CG	TYR	A	345	63.497	50.163	41.314	1.00	28.95
ATOM ·	1703	CD1	TYR	A	345	62.325	50.822	41.684	1.00	30.04
ATOM C	1704	CD2	TYR	A	345	63.412	48.821	40.945	1.00	29.16

ATOM C	1705	CE1	TYR	A	345	61.099	50.165	41.677	1.00	30.92
ATOM C	1706	CE2	TYR	Α	345	62.189	48.154	40.937	1.00	30.52
ATOM C	1707	CZ	TYR	A	345	61.039	48.837	41.300	1.00	31.09
ATOM	1708	ОН	TYR	A	345	59.820	48.205	41.256	1.00	32.41
ATOM N	1709	N	PHE	A	346	67.162	49.281	42.467	1.00	29.90
ATOM C	1710	CA	PHE	A	346	67.795	48.003	42.784	1.00	31.06
ATOM C	1711	С	PHE	A	346	68.170	47.932	44.262	1.00	32.66
ATOM O	1712	0	PHE	A	346	67.958	46.913	44.918	1.00	32.46
ATOM . C	1713	CB	PHE	A	346	69.051	47.814	41.932	1.00	30.74
ATOM C	1714	CG	PHE	A	346	69.844	46.589	42.287	1.00	31.11
ATOM C	1715	CD1	PHE	·A	346	69.329	45.319	ű2.053	1.00	29.91
ATOM C	1716	CD2	PHE	A	346	71.107	46.708	42.861	1.00	32.41
ATOM C	1717	CE1	PHE	A	346	70.061	44.177	42.383	1.00	30.76
ATOM C	1718	CE2	PHE	A	346	71.850	45.572	43.197	1.00	33.67
ATOM C	1719	CZ	PHE	A	346	71.321	44.303	42.954	1.00	32.41
ATOM N	1720	N	GLU	A	347	68.726	49.021	44.782	1.00	33.10
ATOM C	1721	CA	GLU	A	347	69.130	49.072	46.182	1.00	36.04
ATOM C	1722	C	GLU	A	347	67.933	49.020	47.127	1.00	35.98
ATOM O	1723	0	GLU	Α	347	68.032	48.491	48.235	1.00	35.44
ATOM C	1724	СВ	GLU	A	347	69.947	50.340	46.448	1.00	37.89
	1725	CG	GLU	A	3.47	71.259	50.392	45.672	1.00	42.81
ATOM C	1726	CD	GLU	A	347	72.257	49.319	46.102	1.00	46.57
ATOM O	1727	OE1	GLU	A	347	73.243	49.099	45.363	1.00	48.05
ATOM O	1728	OE2	GLU	A	347	72.071	48.702	47.177	1.00	48.54
ATOM N	1729	N	GLU	A	348	66.802	49.560	46.687	1.00	35.06
ATOM C	1730	CA	GLU	A	348	65.603	49.579	47.513	1.00	35.70
ATOM C	1731	C .	GLU	A	348	64.834	48.261	47.511	1.00	35.13
ATOM O	1732	0	GLU	A	348	64.349	47.817	48.551	1.00	34.62

ATOM C	1733	CB ·	GLU	A	348	64.633	50.671	47.043	1.00	37.06
ATOM C	1734	CG	GLU	A	348	65.237	52.044	46.812	1.00	39.63
ATOM C	1735	CD .	GLU	A	3,48	64.207	53.056	46.324	1.00	40.78
MOTA O	1736	OE1	GLU	A	348	63.274	52.662	45.592	1.00	40.73
ATOM O	1737	OE2	GLU	A	348	64.340	54.251	46.660	1.00	43.08
ATOM N	1738	N	THR	A	349	64.727	47.640	46.342	1.00	33.88
ATOM .	1739	CA	THR	A	349	63.948	46.415	46.187	1.00	33.76
ATOM C	1740	C	THR	A	349	64.713	45.121	45.922	1.00	33.08
ATOM O	1741	0	THR	A	349	64.136	44.040	46.007	1.00	33.38
ATOM C	1742	CB	THR	A	349	62.955	46.567	45.029	1.00	33.48
ATOM O	1743	OG1	THR	A	349	63.686	46.612	43.794	1.00	32.62
ATOM C	1744	CG2	THR	A	349	62.147	47.859	45.173	1.00	33.82
ATOM N	1745	N	GLY	A	350	65.991	45.227	45.584	1.00	32.81
ATOM C	1746	CA	GLY	A	350	66.762	44.035	45.283	1.00	31.80
ATOM C	1747	С	GLY	A	350	66.481	43.557	43.865	1.00	31.19
MOTA O	1748	0	GLY	A	350	66.976	42.515	43.440	1.00	31.53
ATOM N	1749	N	ILE	A	351	65.687	44.327	43.125	1.00	30.11
ATOM C	1750	CA	ILE	A	351	65.338	43.982	41.749	1.00	28.23
ATOM C	1751	С	ILE	A	351	66.182	44.775	40.751	1.00	26.97
MOTA O	1752	0	ILE	A	351	66.188	46.005	40.780	1.00	25.49
ATOM C	1753	СВ	ILE	A	351	63.859	44.308	41.442	1.00	30.29
ATOM C	1754	CG1	ILE	A	351	62.934	43.608	42.442	1.00	31.76
ATOM C	1755	CG2	ILE	A	351	63.533	43.901	40.008	1.00	30.03
ATOM C	1756	CD1	ILE	A	351	61.497	44.104	42.383	1.00	33.25
ATOM N	1757	N	TYR	A	352	66.888	44.075	39.872	1.00	25.98
ATOM	1758	CA	TYR	A	352	67.699	44.747	38.862	1.00	25.54
C ATOM C	1759	С	TYR	A	352	66.955	44.707	37.541	1.00	25.29
ATOM O	1760	0	TYR	A	352	66.696	43.631	37.002	1.00	24.79

ATOM C	1761	СВ	TYR	A	352	69.055	44.064	38.674	1.00	26.27
ATOM C	1762	CG	TYR	A	352	69.950	44.807	37.696		25.26
ATOM C	1763	CD1	TYR	A	352	70.741	45.873	38.122	1.00	25.87
ATOM C	1764	CD2	TYR	A	352	69.983	44.464	36.342	1.00	26.91
ATOM C	1765	CE1	TYR	A	352	71.545	46.578	37.235	1.00	25.26
ATOM C	1766	CE2	TYR	A	352	70.788	45.172	35.436	1.00	26.20
ATOM C	1767	CZ	TYR	A	352	71.568	46.226	35.895	1.00	25.73
ATOM O	1768	ОН	TYR	A	352	72.394	46.918	35.030	1.00	24.57
ATOM N	1769	N	ILE	A	353	66.623	45.884	37.016	1.00	24.76
ATOM	1770	CA	ILE	A	353	65.906	45.984	35.754	1.00	24.38
C ATOM C	1771	С	ILE	A	353	66.813	46.507	34.648	1.00	24.63
ATOM O	1772	0	ILE	Α	353 ,	67.263	47.652	34.695	1.00	23.98
ATOM	1773	CB	ILE	A	353	64.697	46.939	35.877	1.00	25.07
C ATOM C	1774	CG1	ILE	A	353	63.745	46.435	36.974	1.00	25.69
ATOM C	1775	CG2	ILE	A	353	63.977	47.030	34.531	1.00	24.50
ATOM C	1776	CD1	ILE	A	353	62.534	47.308	37.205	1.00	25.89
ATOM N	1777	N	PRO	A	354	67.111	45.667	33.642	1.00	24.90
ATOM C	1778	CA	PRO	A	354	67.974	46.100	32.537	1.00	24.20
ATOM C	1779	С	PRO	A	354	67.311	47.244	31.779	1.00	24.12
ATOM O	1780	0 .	PRO	A	354	66.089	47.268	31.641	1.00	24.10
ATOM C	1781	CB	PRO	Α	354	68.085	44.846	31.669	1.00	24.27
ATOM	1782	CG	PRO	A	354	67.941	43.720	32.681	1.00	23.16
C ATOM C	1783	CD	PRO	A	354	66.802	44.229	33.536	1.00	24.40
ATOM N	1784	N	VAL	A	355	68.109	48.191	31.295	1.00	23.66
ATOM C	1785	CA	VAL	A	355	67.556	49.298	30.526	1.00	22.79
MOTA	1786	С	VAL	A	355	68.210	49.322	29.158	1.00	23.11
C ATOM O	1787	0	VAL	A	355	69.359	48.916	28.990	1.00	22.38
ATOM C	1788	СВ	VAL	A	355	67.735	50.671	31.239	1.00	22.02

ATOM C	1789	CG1	VAL	A	355	66.979	50.665	32.555	1.00	22.53
ATOM C	1790	CG2	VAL	A	355	69.209	50.981	31.456		20.21
ATOM	1791	N	CYS	A	356	67.454	49.794	28.178	1.00	23.23
N ATOM C	1792	CA	CYS	A	356	67.906	49.842	26.802	1.00	23.04
ATOM C	1793	С	CYS	Α	356	67.981	51.272	26.287	1.00	23.29
MOTA	1794	0	CYS	Α	356	67.023	52.025	26.414	1.00	22.76
O ATOM C	1795	СВ	CYS	A	356	66.924	49.035	25.940	1.00	25.03
ATOM S	1796	SG	CYS	A	356	67.126	49.192	24.147	1.00	25.41
ATOM	1797	N	SER	A	357	69.126	51.647	25.727	1.00	22.98
N ATOM C	1798	CA	SER	A	357	69.268	52.975	25.148	1.00	22.85
ATOM C	1799	С	SER	A	357	68.771	52.806	23.718	1.00	23.16
ATOM	1800	0	SER	A	357	69.398	52.122	22.913	1.00	22.80
O ATOM C	1801	СВ	SER	A	357	70.724	53.428	25.138	1.00	21.98
ATOM O	1802	OG	SER	A	357	70.813	54.733	24.584	1.00	23.23
ATOM	1803	N	ASP	A	358	67.646	53.441	23.417	1.00	22.79
N ATOM	1804	CA	ASP	A	358 ·	67.020	53.333	22.109	1.00	24.60
C ATOM C	1805	С	ASP	A	358	67.090	54.614	21.279	1.00	25.62
ATOM O	1806	0	ASP	A	358	66.466	55.616	21.617	1.00	25.58
ATOM C	1807	CB	ASP	A	358	65.560	52.900	22.314	1.00	24.15
ATOM C	1808	CG	ASP	A	358	64.776	52.816	21.026	1.00	25.77
ATOM O	1809	OD1	ASP	A	358	65.394	52.717	19.943	1.00	25.59
ATOM .	1810	OD2	ASP	A	358	63.530	52.833	21.111	1.00	25.33
O ATOM N	1811	N	GLY	Α	359	67.860	54.562	20.193	1.00	28.47
ATOM C	1812	CA	GLY	Α	359	67.989	55.702	19.302	1.00	30.93
ATOM C	1813	С	GLY	Α	359	69.129	56.657	19.604 ⁻	1.00	33.00
MOTA O	1814	0	GLY	A	359	69.679	56.665	20.706	1.00	33.66
ATOM N	1815	N	GLY	Α	360	69.490	57.463	18.610	1.00	34.46
ATOM C	1816	CA	GLY	Α	360	70.551	58.434	18.793	1.00	35.68

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ATOM C	1817	C .	GLY	A	360	71.968	57.960	18.533	1.00	36.49
ATOM O	1818	0	GLY	A	360	72.905	58.740	18.671	1.00	38.41
ATOM N	1819	N	ILE	A	361	72.146	56.696	18.169	1.00	36.80
ATOM C	1820	CA	ILE	A	361	73.486	56.186	17.895	1.00	37.13
ATOM C	1821	С	ILE	Α	361	73.885	56.609	16.483	1.00	38.00
MOTA O	1822	0	ILE	A	361	73.275	56.173	15.506	1.00	37.36
ATOM C	1823	CB	ILE	A	361	73.543	54.640	17.980	1.00	37.20
ATOM C	1824	CG1	ILE	A	361	73.123	54.166	19.377	1.00	36.99
ATOM C	1825	CG2	ILE	A	361	74.951	54.153	17.666	1.00	37.15
	1826	CD1	ILE	A	361	74.050	54.607	20.493	1.00	36.40
	1827	N	VAL	A	362	74.898	57.466	16.384	1,00	37.48
ATOM C	1828	CA	VAL	Α	362	75.373	57.940	15.088	1.00	38.82
ATOM C	1829	С	VAL	A	362	76.707	57.292	14.735	1.00	38.61
	1830	0	VAL	A	362	76.916	56.862	13.599	1.00	39.64
ATOM C	1831	CB	VAL	A	362	75.548	59.473	15.082	1.00	39.34
	1832	CG1	VAL	A	362	76.006	59.946	13.701	1.00	41.47
ATOM C	1833	CG2	VAL	A	362	74.241	60.142	15.458	1.00	40.61
ATOM N	1834	N	TYR	A	363	77.600	57.215	15.719	1.00	37.19
ATOM · C	1835	CA	TYR	A	363	78.921	56.624	15.530	1.00	36.38
ATOM C	1836	С	TYR	Α	363	79.131	55.425	16.447	1.00	34.11
ATOM O	1837	0	TYR	A	363	78.471	55.303	17.477	1.00	32.33
ATOM ´	1838	CB	TYR	A	363	80.004	57.661	15.820	1.00	39.61
	1839	CG _.	TYR	A	363	79.918	58.894	14.957	1.00	43.43
ATOM C	1840	CD1	TYR	A	363	79.948	58.795	13.565	1.00	45.21
	1841	CD2	TYR	Α	363	79.824	60.162	15.527	1.00	44.88
ATOM C	1842	CE1	TYR	A	363	79.889	59.933	12.761	1.00	47.51
	1843	CE2	TYR	A	363	79.766	61.308	14.731	1.00	47.32
	1844	CZ	TYR	А	363	79.800	61.184	13.351	1.00	47.96

MOTA O	1845	ОН	TYR	A	363	79.755	62.310	12.556	1.00	49.68
ATOM N	1846	N	ASP	A	364	80.059	54.548	16.079	1.00	32.88
ATOM C	1847	CA	ASP	A	364	80.341	53.375	16.899	1.00	32.27
ATOM C	1848	С	ASP	A	364	80.649	53.733	18.352	1.00	30.99
ATOM O	1849	0	ASP	A	364	80.189	53.050	19.266	1.00	31.26
ATOM C	1850	CB	ASP	Α	364	81.531	52.574	16.351	1.00	34.38
ATOM C	1851	CG	ASP	A	364	81.224	51.867	15.040	1.00	36.34
ATOM O	1852	OD1	ASP	A	364	80.081	51.396	14.850	1.00	37.26
ATOM O	1853	OD2	ASP	A	364	82.147	51.767	14.205	1.00	37.51
ATOM N	1854	N	TYR	A	365	81.421	54.796	18.576	1.00	29.18
ATOM C	1855	CA.	TYR	A	365	81.776	55.153	19.949	1.00	27.62
ATOM	1856	C	TYR	A	365	80.571	55.537	20.796	1.00	27.21
C ATOM O	1857	0	TYR	A	365	80.638	55.497	22.019	1.00	25.96
ATOM C	1858	СВ	TYR	A	365	82.846	56.257	19.982	1.00	28.21
ATOM C	1859	CG	TYR	A	365	82.351	57.679	19.854	1.00	29.19
ATOM	1860	CD1	TYR	A	365	82.157	58.483	20.983	1.00	30.31
C ATOM C	1861	CD2	TYR	A	365	82.135	58.242	18.602	1.00	30.72
ATOM C	1862	CE1	TYR	A	365	81.765	59.824	20.854	1.00	31.27
ATOM C	1863	CE2	TYR	A	365	81.746	59.568	18.464	1.00	32.19
ATOM C	1864	CZ	TYR	A	365	81.565	60.353	19.587	1.00	32.87
ATOM O	1865	ОН	TYR	A	365	81.178	61.664	19.418	1.00	3.5.54
MOTA	1866	N	HIS	A	366	79.465	55.896	20.149	1.00	25.79
N ATOM C	1867	CA	HIS	A	366	78.253	56.229	20.888	1.00	26.00
AŢOM C	1868	С	HIS	A	366	77.757	54.963	21.582	1.00	25.36
ATOM O	1869	0	HIS	A	366	77.091	55.035	22.616	1.00	24.64
ATOM C	1870	СВ	HIS	A	366	77.160	56.760	19.956	1.00	26.79
ATOM C	1871	CG	HIS	A	366	77.409	58.148	19.455	1.00	28.37
ATOM N	1872	ND1	HIS	A	366	78.402	58.958	19.963	1.00	29.63

ATOM C	1873	CD2	HIS	A	366	76.774	58.880	18.510	1.00	28.28
ATOM C	1874	CE1	HIS	A	366	78.368	60.129	19.352	1.00	27.78
ATOM N	1875	NE2	HIS	A	366	77.390	60.108	18.466	1.00	29.94
ATOM N	1876	N	MET	A	367	78.067	53.803	21.000	1.00	24.84
ATOM C	1877	CA	MET	A	367	77.663	52.530	21.602	1.00	25.78
ATOM C	1878	С	MET	A	367	78.401	52.385	22.927	1.00	24.73
ATOM O	1879	0	MET	A	367	77.816	52.063	23.950	1.00	23.39
ATOM C	1880	СВ	MET	A	367	78.035	51.343	20.704	1.00	26.59
ATOM C	1881	CG	MET	A	367	77.291	51.272	19.369	1.00	30.31
ATOM S	1882	SD	MET	A	367	77.849	49.839	18.398	1.00	32.89
ATOM C	1883	CE	MET	Α	367	77.037	50.144	16.824	1.00	32.21
ATOM N	1884	N	THR	A	368	79.707	52.611	22.881	1.00	24.71
ATOM C	1885	CA	THR	A	368	80.547	52.510	24.064	1.00	24.03
ATOM C	1886	С	THR	A	368	80.063	53.484	25.135	1.00	23.45
ATOM O	1887	0	THR	A	368	79.985	53.133	26.306	1.00	23.07
ATOM C	1888	CB	THR	A	368	82.006	52.816	23.701	1.00	24.76
ATOM O	1889	OG1	THR	A	368	82.349	52.081	22.518	1.00	24.31
ATOM C	1890	CG2	THR	A	368	82.942	52.411	24.835	1.00	24.75
ATOM N	1891	N	LEU	A	369	79.744	54.710	24.731	1.00	23.16
ATOM C	1892	CA	LEU	A	369	79.249	55.722	25.666	1.00	24.00
ATOM C	1893	С	LEU	A	369	77.939	55.308	26.335	1.00	23.72
ATOM O	1894	0	LEU	A	369	77.797	55.411	27.551	1.00	23.10
ATOM C	1895	СВ	LEU	A	369	79.033	57.057	24.947	1.00	24.17
ATOM C	1896	CG	LEU	A	369	80.281	57.884	24.624	1.00	26.48
ATOM C	1897	CD1	LEU	A	369	79.897	59.087	23.772	1.00	26.96
ATOM C	1898	CD2	LEU	A	369	80.943	58.342	25.926	1.00	26.87
ATOM N	1899	N	ALA	A	370	76.986	54.837	25.533	1.00	22.35
ATOM C	1900	CA	ALA	A	370	75.686	54.424	26.056	1.00	23.03

ATOM	1901	С	ALA	Α	370	75.857	53.331	27.108	1.00	22.11
C ATOM	1902	0	ALA	Α	370	75.228	53.361	28.162	1.00	22.10
O ATOM	1903	СВ	ALA	Α	370	74.803	53.917	24.917	1.00	21.13
C ATOM	1904	N	LEU	Α	371	76.707	52.361	26.805	1.00	21.79
N ATOM	1905	CA	LEU	Α	371	76.960	51.261	27.726	1.00	22.39
C ATOM	1906	С	LEU	A	371	77.685	51.777	28.972	1.00	21.96
C ATOM	1907	0	LEU	A	371	77.355	51.399	30.098	1.00	21.20
O ATOM	1908	СВ	LEU	A	371	77.803	50.186	27.030	1.00	21.70
C ATOM	1909	CG	LEU	A	371	77.170	49.473	25.820	1.00	22.99
C ATOM	1910	CD1	LEU	A	371	78.221	48.634	25.112	1.00	24.60
C ATOM C	1911	CD2	LEU	A	371	76.009	48.591	26.270	1.00	23.11
MOTA	1912	N	ALA	A	372	78.680	52.636	28.770	1.00	21.79
N ATOM	1913	CA	ALA	A	372	79.437	53.182	29.894	1.00	21.89
C ATOM	1914	С	ALA	A	372	78.534	53.993	30.812	1.00	23.49
C ATOM	1915	0	ALA	A	372	78.720	54.004	32.032	1.00	22.41
O ATOM	1916	CB	ALA	A	372	80.585	54.052	29.387	1.00	22.98
C ATOM N	1917	N	MET	A	373	77.550	54.675	30.231	1.00	22.86
ATOM C	1918	CA	MET	A	373	76.632	55.471	31.039	1.00	23.45
ATOM C	1919	С	MET	A	373	75.650	54.609	31.829	1.00	23.67
ATOM O	1920	Ο.	MET	Α	373	74.913	55.119	32.665	1.00	24.88
ATOM C	1921	CB	MET	Α	373	75.884	56.474	30.159	1.00	23.86
ATOM C	1922	CG	MET	Α	373	76.792	57.571	29.612	1.00	25.21
ATOM S	1923	SD	MET	Ά	373	75.984	58.618	28.385	1.00	26.48
ATOM C	1924	CE	MET	A	373	77.324	59.787	28.016	1.00	26.43
ATOM N	1925	N	GLY	Α	. 374	75.635	53.302	31.572	1.00	23.45
ATOM C	1926	CA	GLY	A	374	74.745	52.443	32.332	1.00	22.34
ATOM C	1927	С	GLY	Α	. 374	73.740	51.597	31.573	1.00	22.77
ATOM O	1928	0	GLY	A	. 374	73.118	50.714	32.162	1.00	23.42

ATOM N	1929	N	ALA	A	375	73.560	51.851	30.283	1.00	22.25
ATOM C	1930	CA	ALA	A	375	72.614	51.051	29.509	1.00	22.62
ATOM C	1931	С	ALA	Α	375	73.143	49.625	29.389	1.00	23.21
ATOM O	1932	0	ALA	A	375	74.329	49.416	29.134	1.00	23.32
ATOM C	1933	CB	ALA	A	375	72.418	.51.652	28.120	1.00	22.37
ATOM N	1934	N	ASP	A	376	72.263	48.645	29.580	1.00	·22.37
ATOM C	1935	CA	ASP	A	376	72.661	47.244	29.478	1.00	23.13
ATOM C	1936	С	ASP	A	376	72.750	46.840	28.012	1.00	23.56
ATOM O	1937	0	ASP	A	376	73.624	46.064	27.624	1.00	23.83
ATOM C	1938	СВ	ASP	A	376	71.665	46.377	30.241	1.00	23.78
ATOM C	1939	CG	ASP	A	376	71.596	46.756	31.706	1.00	24.06
ATOM O	1940	OD1	ASP	A	376	72.420	46.246	32.499	1.00	25.54
ATOM O	1941	OD2	ASP	A	376	70.734	47.586	32.062	1.00	23.75
ATOM N	1942	N	PHE	A	377	71.841	47.355	27.193	1.00	23.34
ATOM C	1943	CA	PHE	A	377	71.904	47.076	25.768	1.00	23.57
ATOM C	1944	С	PHE	A	377	71.414	48.262	24.948	1.00	23.98
ATOM	1945	0	PHE	A	377	70.882	49.228	25.490	1.00	23.49
O ATOM C	1946	СВ	PHE	A	377	71.168	45.778	25.385	1.00	23.30
ATOM C	1947	CG	PHE	A	377	69.758	45.684	25.887	1.00	24.76
ATOM C	1948	ÇD1	PHE	A	3,77	69.495	45.318	27.203	1.00	26.77
ATOM	1949	CD2	PHE	A	377	68.688	45.900	25.025	1.00	24.49
ATOM C	1950	CE1	PHE	A	377	68.180	45.163	27.652	1.00	26.00
ATOM	1951	CE2	PHE	A	377	67.370	45.747	25.465	1.00	25.78
C ATOM C	1952	CZ	PHE	A	377	67.118	45.379	26.777	1.00	25.44
MOTA N	1953	N	ILE	A	378	71.610	48.181	23.639	1.00	23.02
ATOM C	1954	CA	ILE	A	378	71.278	49.271	22.738	1.00	23.35
ATOM C	1955	С	ILE	A	378	70.335	48.846	21.621	1.00	23.49
ATOM O	1956	0	ILE	A	378	70.502	47.778	21.045	1.00	24.62

ATOM C	1957	CB	ILE A	A	378	72.592	49.816	22.107	1.00	23.26
ATOM C	1958	CG1	ILE A	A	378	73.571	50.202	23.227	1.00	24.03
ATOM	1959	CG2	ILE	A	378	72.306	51.011	21.192	1.00	24.70
C ATOM	1960	CD1	ILE .	A	378	75.017	50.325	22.756	1.00	26.63
C ATOM	1961	N	MET .	A	379	69.335	49.675	21.331	1.00	23.56
N ATOM	1962	CA	MET .	A	379	68.418	49.374	20.238	1.00	23.95
C ATOM	1963	С	MET .	A	379	68.755	50.340	19.109	1.00	24.40
C ATOM	1964	0	MET	A	379	68.915	51.540	19.338	1.00	23.43
O ATOM	1965	СВ	MET	Α	379	66.952	49.551	20.661	1.00	24.65
C ATOM	1966	CG	MET	A	379	65.968	49.319	19.508	1.00	24.74
C ATOM	1967	SD	MET	A	379	64.236	49.290	19.988	1.00	26.39
S ATOM	1968	CE	MET	Α	379	64.115	47.609	20.644	1.00	27.00
C ATOM	1,969	N	LEU	A	380	68.881	49.815	17.896	1.00	24.73
N ATOM	1970	CA	LEU	Α	380	69.216	50.642	16.744	1.00	25.39
C ATOM	1971	С	LEU	Α	380	68.334	50.345	15.545	1.00	25.28
C ATOM	1972	0	LEU	A	380	67.952	49.197	15.316	1.00	25.31
O ATOM	1973	СВ	LEU	Α	380	70.673	50.421	16.329	1.00	26.35
C ATOM	1974	CG	LEU	A	380	71.756	50.577	17.403	1.00	27.26
C ATOM	1975	CD1	LEÙ	Α	380	71.877	49.280	18.189	1.00	29.84
C ATOM	1976	CD2	LEU	Α	380	73.081	50.896	16.740	1.00	28.50
C ATOM	1977	N	GLY	A	381	68.034	51.388	14.778	1.00	25.23
N ATOM	1978	CA	GLY	A	381	67.221	51.232	13.584	1.00	27.24
C ATOM C	1979	С	GLY	A	381	68.057	51.437	12.331	1.00	27.95
ATOM O	1980	Ó	GLY	A	381	68.330	50.493	11.592	1.00	28.13
ATOM	1981	N	ARG	A	382	68.473	52.680	12.107	1.00	29.76
N ATOM	1982	CA	ARG	A	382	69.279	53.061	10.945	1.00	31.76
C ATOM C	1983	С	ARG	A	382	70.494	52.150	10.748	1.00	32.08
ATOM O	1984	0	ARG	A	382	70.778	51.702	9.632	1.00	30.90

ATOM C	1985	СВ	ARG	A	382	69.744	54.510	11.109	1.00	34.27
ATOM C	1986	CG	ARG	A	382	70.563	55.063	9.952	1.00	39.22
ATOM	1987	CD	ARG	A	382	71.207	56.388	10.339	1.00	42.02
C ATOM N	1988	NE	ARG	A	382	72.131	56.221	11,460	1.00	45.45
ATOM C	1989	CZ	ARG	A	382	73.260	55.518	11.399	1.00	47.01
ATOM	1990	NH1	ARG	A	382	73.610	54.920	10.267	1.00	48.07
N ATOM N	1991	NH2	ARG	Α	382	74.033	55.399	12.471	1.00	47.88
ATOM N	1992	N	TYR	A	383	71.208	51.883	11.838	1.00	30.72
ATOM	1993	CA	TYR	A	383	72.395	51.032	11.804	1.00	30.04
C ATOM C	1994	С	TYR	A	383	72.136	49.699	11.098	1.00	29.56
ATOM O	1995	0	TYR	A	383	72.922	49.272	10.252	1.00	30.58
ATOM	1996	СВ	TYR	A	383	72.876	50.761	13.234	1.00	29.03
C ATOM	1997	CG	TYR	Α	383	74.100	49.878	13.329	1.00	28.59
C ATOM C	1998	CD1	TYR	A	383	75.381	50.413	13.201	1.00	29.36
ATOM C	1999	CD2	TYR	A	383	73.975	48.505	13.538	1.00	28.86
MOTA	2000	CE1	TYR	A	383	76.509	49.602	13.280	1.00	29.26
C ATOM C	2001	CE2	TYR	A	383	75.097	47.683	13.617	1.00	28.40
ATOM C	2002	CZ	T:YR	A	383	76.360	48.240	13.486	1.00	28.60
ATOM O	2003	OH	TYR	Α	383	77.475	47.437	13.551	1.00	28.39
ATOM N	2004	N	PHE	A	384	71.034	49.048	11.452	1.00	29.09
ATOM C	2005	CA.	PHE	A	384	. 70.679	47.757	10.872	1.00	29.81
ATOM	2006	С	PHE	A	384 .	69.991	47.843	9.510	1.00	30.44
C ATOM O	2007	0	PHE	A	384	70.102	46.922	8.701	1.00	30.80
ATOM C	2008	CB	PHE	A	384	69.785	46.976	11.842	1.00	29.45
ATOM C	2009	CG	PHE	Α	384	70.511	46.460	13.057	1.00	28.89
ATOM C	2010	CD1	PHE	Α	384	71.469	45.455	12.936	1.00	28.54
ATOM C	2011	CD2	PHE	A	384	70.237	46.980	14.322	1.00	28.04
ATOM C	2012	CE1	PHE	A	384	72.146	44.973	14.054	1.00	28.18

ATOM C	2013	CE2	PHE	Α	384	70.905	46.506	15.446	1.00	27.99
ATOM C	2014	CZ	PHE	A	384	71.864	45.500	15.313	1.00	27.33
ATOM N	2015	N	ALA	A	385	69.286	48.940	9.258	1.00	31.37
ATOM C	2016	CA	ALA	Ą	385	68.582	49.118	7.991	1.00	32.83
ATOM C	2017	С	ALA	A	385	69.530	49.082	6.795	1.00	33.97
ATOM O	2018	0	ALA	A	385	69.137	48.700	5.694	1.00	34.53
ATOM C	2019	СВ	ALA	A	385	67.815	50.433	8.004	1.00	31.76
ATOM N	2020	N	ARG	A	386	70.779	49.482	7.018	1.00	35.25
ATOM C	2021	CA	ARG	A	386	71.786	49.508	5.960	1.00	35.62
ATOM C	2022	С	ARG	A	386	72.237	48.120	5.511	1.00	36.16
ATOM O	2023	0	ARG	A	386	72.911	47.986	4.488	1.00	35.70
ATOM C	2024	CB	ARG	A	386	73.027	50.272	6.428	1.00	36.74
ATOM C	2025	CG	ARG	A	386	72.816	51.708	6.857	1.00	38.32
ATOM C	2026	CD	ARG	Α	386	74.090	52.191	7.536	1.00	40.83
ATOM N	2027	NE	ARG	A	386	74.477	51.251	8.585	1.00	42.25
MOTA	2028	CZ	ARG	A	386	75.726	51.019	8.973	1.00	42.05
C ATOM N	2029	NH1	ARG	A	386	76.737	51.661	8.401	1.00	41.85
ATOM N	2030	NH2	ARG	A	386	75.960	50.131	9.930	1.00	41.04
MOTA	2031	N	PHE	A	387	71.875	47.088	6.266	1.00	36.71
N ATOM C	2032	CA	PHE	A	387	72.309	45.740	5.928	1.00	37.28
ATOM C	2033	Ċ	PHE	A	387	71.442	44.973	4.938	1.00	38.78
MOTA	2034	0	PHE	A	387	70.249	45.233	4.779	1.00	38.34
O ATOM C	2035	СВ	PHE	A	387	72.483	44.900	7.202	1.00	37.27
ATOM C	2036	CG	PHE	A	387	73.397	45.524	8.222	1.00	36.45
MOTA	2037	CD1	PHE	A	387	74.507	46.263	7.826	1.00	36.98
C ATOM C	2038	CD2	PHE	A	387	73.152	45.364	9.584	1.00	36.75
ATOM C	2039	CE1	PHE	Α	38,7	75.362	46.838	8.771	1.00	36.90
ATOM C	2040	CE2	PHE	A	387	73.998	45.931	10.536	1.00	35.15

ATOM C	2041	CZ	PHE	A	387	75.104	46.670	10.130	1.00	36.18
ATOM N	2042	N	GLU	A	388	72.081	44.013	4.280	1.00	39.94
ATOM	2043	CA	GLU	A	388	71.442	43.155	3.294	1.00	41.27
C ATOM C	2044	С	GLU	A	388	70.225	42.453	3.878	1.00	41.01
ATOM O	2045	0	GLU	Α	388	69.216	42.268	3.195	1.00	40.68
ATOM C	2046	СВ	GLU	A	388	72.453	42.111	2.809	1.00	42.64
ATOM C	2047	CG	GLU	A	388	71.901	41.064	1.853	1.00	46.30
ATOM C	2048	CD	GLU	A	388	71.435	41.660	0.542	1.00	47.81
ATOM	2049	OE1	GLU	A	388	72.184	42.474	-0.033	1.00	49.41
O ATOM O	2050	OE2	GLU	À	388	70.326	41.310	0.081	1.00	50.01
ATOM	2051	N	GLU	A	389	70.317	42.076	5.150	1.00	40.05
N ATOM C	2052	CA	GLU	A	389	69.230	41.365	5.807	1.00	39.60
ATOM	2053	С	GLU	A	389	68.002	42.182	6.200	1.00	39.15
C ATOM O	2054	0	GLU	A	389	67.006	41.605	6.628	1.00	38.91
ATOM C	2055	СВ	GLU	A	389	69.758	40.611	7.031	1.00	39.09
ATOM	2056	CG	GLU	A	389	70.789	39.544	6.685	1.00	38.57
C ATOM C	2057	CD	GLU	A	389	72.223	40.049	6.746	1.00	37.83
ATOM O	2058	OE1	GLU	A	389	72.453	41.267	6.600		38.50
ATOM O	2059	OE2	GLU	A	389	73.128	39.216	6.929	1.00	37.79
ATOM N	2060-	N			390	68.057			-	39.34
ATOM	2061	CA	SER	A	390	66.879	44.303	6.417	1.00	41.26
C ATOM C	2062	С	SER	A	390	65.839	43.965	5.343	1.00	42.43
ATOM	2063	0	SER	A	390	66.193	43.713	4.192	1.00	42.09
O ATOM . C	2064	СВ	SER	A	390	67.194	45.799	6.408	1.00	40.53
MOTA	2065	OG ·	SER	A	390	67.514	46.256	5.111	1.00	44.02
O ATOM N	2066	N	PRO	Α	391	64.547	43.961	5.707	1.00	43.44
ATOM C	2067	CA	PRO	Α	391	63.452	43.639	4.780	1.00	44.56
ATOM C	2068	Ċ	PRO	A	391	63.123	44.645	3.678	1.00	45.93

ATOM O	2069	0	PRO ·	A	391	62.217	44.409	2.876	1.00	46.82
ATOM C	2070	CB	PRO	A	391	62.273	43.423	5.722	1.00	44.41
ATOM C	2071	CG	PRO	A	391	62.526	44.459	6.77 <b>7</b>	1.00	43.55
ATOM C	2072	CD	PRO	A	391	64.018	44.320	7.036	1.00	42.66
ATOM N	2073	N	THR	A	392	63.848	45.755	3.623	1.00	46.64
ATOM C	2074	CA	THR	A	392	63.573	46.767	2.612	1.00	47.66
ATOM C	2075	С	THR	A	392	64.258	46.479	1.282	1.00	49.02
ATOM O	2076	0	THR	A	392	65.106	45.591	1.182	1.00	49.01
ATOM C	2077	СВ	THR	A	392	64.000	48.162	3.092	1.00	47.33
ATOM O	2078	OG1	THR	A	392	65.419	48.188	3.286	1.00	47.34
ATOM C	2079	CG2	THR	A	392	63.301	48.505	4.403	1.00	47.28
ATOM N	2080	N	ARG	A	393	63.883	47.240	0.260	1.00	50.71
ATOM C	2081	CA	ARG	A	393	64.456	47.061	-1.066	1.00	52.75
ATOM C	2082	С	ARG	A	393	65.795	47.757	-1.219	1.00	53.23
ATOM O	2083	0	ARG	A	393 -	65.993	48.876	-0.743	1.00	52.80
ATOM C	2084	CB	ARG	A	393	63.513	47.595	-2.146	1.00	53.96
ATOM C	2085	CG	ARG	A	393	62.189	46.865	-2.283	1.00	56.12
ATOM C	2086	CD	ARG	A	393	61.493	47.344	-3.545	1.00	57.41
ATOM N	2087	NE	ARG	A	393	61.452	48.802	-3.587	1.00	59.49
ATOM C	2088	CZ	ARG	A	393	61.357	49518	-4.702	1.00	60.61
ATOM N	2089	NH1	ARG	A	393	61.291	48.913	-5.881	1.00	61.26
ATOM ·	2090	NH2	ARG	A	393	61.337	50.842	-4.636	1.00	61.38
ATOM N	2091	N	LYS	A	394	66.713	47.077	-1894	1.00	54.19
ATOM C	2092	ÇA	LYS	A	394	68.031	47.621	-2.159	1.00	55.50
ATOM C	2093	С	LYS	A	394	67.894	48.335	-3.497	1.00	56.45
ATOM O	2094	0	LYS	A	394	67.683	47.692	-4.524	1.00	57.12
ATOM C	2095	СВ	LYS	A	394 .	69.053	46.492	-2.277	1.00	55.00
ATOM C	2096	CG	LYS	A	394	70.490	46.968	-2.348	1.00	55.09

ATOM C	2097	CD	LYS	A	394	71.417	45.863	-2.824	1.00	54.69
ATOM C	2098	CE	LYS	A	394	71.338	44.636	-1.939	1.00	54.30
ATOM N	2099	NZ	LYS	A	394	72.230	43.557	-2.442	1.00	53.86
ATOM N	2100	N	VAL	A	395	67.993	49.659	-3.485	1.00	57.53
ATOM C	2101	CA	VAL	A	395	67.860	50.432	-4.712	1.00	58.92
ATOM C	2102	С	VAL	A	395	69.139	51.181	-5.061	1.00	60.04
ATOM O	2103	0	VAL	A	395	69.813	51.718	-4.183	1.00	59.84
ATOM C	2104	СВ	VAL	A	395	66.704	51.448	-4.603	1.00	59.01
ATOM .	2105	CG1	VAL	Α	395	65.392	50.713	-4.362	1.00	58.97
ATOM C	2106	CG2	VAL	A	395	66.977	52.433	-3.476	1.00	58.87
ATOM N	2107	N	THR	A	396	69.467	51.213	-6.350	1.00	61.16
ATOM	2108	CA	THR	A	396	70.668	51.896	-6.818	1.00	62.32
C ATOM C	2109	С	THR	A	396	70.335	53.283	-7.351	1.00	63.18
ATOM O	2110	0	THR	A	396	69.646	53.421	-8.363	1.00	63.24
ATOM C	2111	CB	THR	A	396	71.367	51.099	-7.934	1.00	62.19
ATOM O	2112	OG1	THR	A	396	71.668	49.780	-7.464	1.00	62.83
ATOM C	2113	CG2	THR	A	396	72.662	51.785	-8.343	1.00	62.42
ATOM N	2114	N	ILE	A	397	70.834	54.305	-6.665	1.00	64.15
ATOM C	2115	CA	ILE	Α	397	70.598	55.689	-7.055	1.00	65.10
ATOM C	2116	С	ILE	A	397	71.899	56.356	-7.499	1.00	65.47
MOTA	2117	0	ILE	A	397	72.866	56.415	-6.741	1.00	65.96
O ATOM C	2118	СВ	ILE	A	397	70.003 -	56.495	-5.884	1.00	65.41
ATOM C	2119	CG1	ILE	A	397	68.709	55.833	-5.404	1.00	65.63
ATOM C	2120	CG2	ILE	A	397	69.736	57.930	-6.320	1.00	65.84
ATOM C	2121	CD1	ILE	A	397	68.079	56.509	-4.203	1.00	66.02
ATOM N	2122	N	ASN	A	398	71.909	56.854	-8.732	1.00	65.71
ATOM C	2123	CA	ASN	A	398	73.073	57.526	-9.307	1.00	65.41
ATOM C	2124	C	ASN	A	398	74.417	56.895	-8.945	1.00	64.56

ATOM	2125	0	ASN	A	398	75.353	57.592	-8.551	1.00	64.63
O ATOM C	2126	CB	ASN	A	398	73.079	59.008	-8.910	1.00	66.44
ATOM C	2127	CG	ASN	A	398	73.115	59.215	-7.405	1.00	67.59
ATOM O	2128	OD1	ASN	A	398	74.046	58.779	-6.725	1.00	68.20
ATOM N	2129	ND2	ASN	A	398	72.099	59.891	-6.878	1.00	67.87
ATOM N	2130	Ν -	GLY	A	399	74.508	55.576	-9.082	1.00	63.47
ATOM	2131	CA	GLY	Α	399	75.751	54.886	-8.779	1.00	61.85
C ATOM C	2132	C	GLY	Α	399	75.918	54.443	-7.338	1.00	60.93
MOTA	2133	0	GLY	A	399	76.854	53.709	-7.016	1.00	61.23
O ATOM	2134	N	SER	A	400	75.019	54.882	-6.464	1.00	59.70
N ATOM C	2135	CA	SER	A	400	75.096	54.511	-5.056	1.00	57.96
ATOM C	2136	С	SER	A	400	73.973	53.577	-4.634	1.00	56.49
ATOM	2137	0	SER	A	400	72.793	53.898	-4.774	1.00	56.56
O ATOM C	2138	СВ	SER	Α	400	75.079	55.761	-4.174	1.00	57.95
ATOM O	2139	OG	SER	A	400	76.286	56.488	-4.305	1.00	58.53
MOTA	2140	N	VAL	A	401	74.351	52.414	-4.118	1.00	54.54
N ATOM C	2141	CA	VAĻ	A	401	73.383	51.431	-3.662	1.00	52.89
ATOM C	2142	С	VAL	A	401	72.864	51.864	-2.293	1.00	52.23
ATOM	2143	0	VAL	A	401	73.637	52.020	-1.344	1.00	51.54
O ATOM	2144	CB	VAL	A	401	74.027	50.038	-3.550	1.00	52.97
ATOM C	2145	CG1	VAL	A	401	72.986	49.012	-3.153	1.00	52.38
MOTA	2146	CG2	VAL	A	401	74.670	49.660	-4.876	1.00	52.77
C ATOM N	2147	N	MET	A	402	71.554	52.066	-2.201	1.00	50.74
ATOM C	2148	CA	MET	A	402	70.933	52.493	-0.954	1.00	49.56
MOTA	2149	C	MET	A	402	69.878	51.490	-0.509	1.00	48.15
C ATOM	2150	0	MET	A	402	69.533	50.563	-1.243	1.00	47.53
O ATOM C	2151	СВ	MET	A	402	70.255	53.855	-1.138	1.00	50.70
ATOM C	2152	CG	MET	A	402	71.080	54.897	-1.873	1.00	51.69

ATOM S	2153	SD	MET	A	402	72.539	55.428	-0.974	1.00	54.36
ATOM C	2154	CE	MET	A	402	71.840	56.729	0.054	1.00	52.69
ATOM	2155	N	LYS	A	403	69.380	51.683	0.708	1.00	45.93
N ATOM C	2156	CA	LYS	Α	403	68.325	50.843	1.258	1.00	43.52
ATOM C	2157	С	LYS	A	403	67.270	51.792	1.806	1.00	42.26
MOTA	2158	0	LYS	A	403	67.598	52.853	2.336	1.00	41.26
O ATOM C	2159	СВ	LYS	A	403	68.856	49.937	2.373	1.00	43.98
ATOM C	2160	CG	LYS	A	403	69.833	48.880	1.887	1.00	43.45
ATOM	2161	CD	LYS	A	403	69.570	47.521	2.524	1.00	43.42
C ATOM C	2162	CE	LYS	A	403	68.229	46.950	2.087	1.00	42.68
ATOM	2163	NZ	LYS	A	403	68.000	45.572	2.601	1.00	40.87
N ATOM	2164	N	GLU	Δ	404	66.003	51.425	1.659	1.00	41.41
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ATOM C	2165	CA	GLU	A	404	64.927	52.275	2.144	1.00	41.08
ATOM C	2166	С	GLU	A	404	64.881	52.222	3.661	1.00	39.67
ATOM	2167	0	GLU	A	404	65.181	51.192	4.265	1.00	38.02
O ATOM C	2168 [°]	СВ	GLU	A	404	63.578	51.809	1.606	1.00	42.91
ATOM C	2169	CG	GLU	A	404	63.610	51.221	0.214	1.00	46.16
ATOM	2170	CD	GĻŪ	A	404	62.230	50.819	-0.252	1.00	47.92
C ATOM O	2171	OE1	GLU	A	404	61.469	51.711	-0.685	1.00	48.56
ATOM O	2172	OE2	GLU	A	404	61.901	49.615	-0.167	1.00	49.37
ATOM	2173	N	TYR	A	405	64.496	53.335	4.271	1.00	38.76
N ATOM C	2174	CA	TYR	Α	405	64.390	53.402	5.717	1.00	38.34
ATOM C	2175	С	TYR	A	405	63.347	54.438	6.094	1.00	37.84
MOTA O	2176	0	TYR	A	405	63.499	55.622	5.796	1.00	38.50
ATOM C	2177	CB	TYR	A	405	65.736	53.770	6.344	1.00	37.72
ATOM C	2178	CG	TYR	A	405	65.698	53.826	7.855	1.00	37.96
ATOM	2179	CD1	TYR	A	405	65.285	52.723	8.602	1.00	36.71
C ATOM C	2180	CD2	TYR	Α	405	66.072	54.982	8.539	1.00	38.07

ATOM C	2181	CE1	TYR	A	405	65.245	52.770	9.9	95	1.00	37.68
ATOM C	2182	CE2	TYR	A	405	66.036	55.038	9.9	31	1.00	38.31
ATOM	2183	CZ	TYR	A	405	65.621	53.929	10.6	50	1.00	37.39
C ATOM O	2184	ОН	TYR	A	405	65.577	53.987	12.0	24	1.00	38.38
ATOM N	2185	N	TRP	A	406	62.287	53.986	6.7	52	1.00	36.25
ATOM C	2186	CA	TRP	Α	406	61.221	54.885	7.1	60	1.00	35.74
ATOM C	2187	С	TRP	A	406	60.829	54.630	8.6	80	1.00	35.35
ATOM O	2188	0	TRP	Α	406	60.906	53.499	9.0	92	1.00	34.84
ATOM C	2189	СВ	TRP	A	406	60.013	54.712	6.2	26	1.00	34.90
ATOM C	2190	CG	TRP	A	406	59.374	53.345	6.2	57	1.00	33.53
ATOM C	2191	CD1	TRP	A	406	58.389	52.920	7.1	00	1.00	33.84
ATOM C	2192	CD2	TRP	A	406	59.679	52.232	5.4	05	1.00	34.08
ATOM N	2193	NE1	TRP	A	406	58.059	51.615	6.8	26	1.00	34.02
ATOM C	2194	CE2	TRP	A	406	58.835	51.167	5.7	91	1.00	33.93
ATOM C	2195	CE3	TRP	A	406	60.584	52.031	4.3	51	1.00	35.20
MOTA	2196	CZ2	TRP	A	406	58.866	49.916	5.1	60	1.00	34.01
C ATOM C	2197	CZ3	TRP	A	406	60.615	50.784	3.7	22	1.00	35.05
ATOM C	2198	CH2	TRP	A	406	59.758	49.744	4.1	.32	1.00	34.39
ATOM	2199	N	GLY	A	407	60.421	55.691	9.2	95	1.00	36.13
N ATOM C	2200	CA	GLY	A	407 .	60.023	55.569	10.6	85	1.00	36.66
ATOM C	2201	С	GLY	A	407	58.630	54.991	10.8	340	1.00	37.56
MOTA	2202	0	GLY	A	407	57.835	54.989	9.8	399	1.00	36.82
O ATOM N	2203	N.	GLU	A	408	58.331	54.495	12.0	35	1.00	37.65
ATOM C	2204	CA	GLU	Α	408	57.022	53.917	12.3	316	1.00	38.92
ATOM C	2205	С	GLU	A	408	55.950	54.998	12.3	390	1.00	40.20
ATOM O	2206	0	GLU	Α	408	54.756	54.704	12.3	37 ⁻ 4	1.00	40.37
ATOM C	2207	СВ	GLU	Α	408	57.071	53.141	13.6	531	1.00	38.51
ATOM C	2208	CG	GLU	Α	408	57.848	51.845	13.5	535	1.00	37.66

ATOM C	2209	CD	GLU	A	408	57.167	50.834	12.625	1.00	37.31
ATOM O	2210	OE1	GLU	A	408	56.048	50.392	12.960	1.00	37.35
MOTA	2211	OE2	GLU	A	408	57.748	50.482	11.578	1.00	35.96
O ATOM N	2212	N	GLY	A	409	56.387	56.249	12.464	1.00	41.46
ATOM C	2213	CA	GLY	Α	409	55.455	57.358	12.544	1.00	43.94
ATOM C	2214	С	GLY	Α	409	55.111	57.955	11.193	1.00	45.38
ATOM O	2215	0	GLY	A	409	54.268	58.844	11.105	1.00	45.63
ATOM N	2216	N	SER	A	410	55.762	57.473	10.138	1.00	46.93
ATOM	2217	CA	SER	A	410	55.499	57.977	8.795	1.00	48.89
C ATOM C	2218	С	SER	A	410	54.184	57.394	.8.293	1.00	50.59
ATOM O	2219	0	SER	A	410	53.798	56.292	8.683	1.00	49.70
ATOM	2220	СВ	SER	Α	410	56.633	57.587	7.840	1.00	48.74
C ATOM O	2221	OG	SER	A	410	56.645	56.189	7.595	1.00	49.10
ATOM N	2222	N	SER	A	411	53.495	58.137	7.433	1.00	52.78
ATOM	2223	CA	SER	A	411	52.224	57.674	6.890	1.00	55.38
C ATOM C	2224	С	SER	A	411	52.436	56.350	6.172	1.00	56.75
ATOM O	2225	0	SER	A	411	51.559	55.487	6.154	1.00	57.17
ATOM C	2226	CB	SER	A	411	51.656	58.710	5.917	1.00	56.02
ATOM O	2227	OG	SER	A	411	52.569	58.984	4.868	1.00	56.98
ATOM N	2228	N	ARG	A	412	53.621	56.195	5.591	1.00	58.21
ATOM	2229	CA	ARG	A	412	53.976	54.985	4.862	1.00	59.73
C ATOM C	2230	С	ARG	A	412	53.968	53.730	5.735	1.00	60.68
ATOM O	2231	0	ARG	A	412	54.038	52.616	5.217	1.00	60.45
ATOM C	2232	CB	ARG	A	412	55.362	55.157	4.227	1.00	59.28
ATOM C	2233	CG	ARG	A	412	55.870	53.925	3.502	1.00	59.26
ATOM C	2234	CD	ARG	A	412	57.209	54.168	2.824	1.00	58.44
ATOM N	2235	NE	ARG	A	412	57.669	52.964	2.141	1.00	57.93
ATOM C	2236	CZ	ARG	A	412	58.797	52.874	1.445	1.00	57.94

ATOM N	2237	NH1	ARG	A	412	59.601	53.923	1.330	1.00	57.62
ATOM N	2238	NH2	ARG	A	412	59.120	51.727	0.863	1.00	58.08
MOTA	2239	N	ALA	A	413	53.865	53.902	7.050	1.00	62.54
N ATOM C	2240	CA	ALA	A	413	53.886	52.756	7.958	1.00	63.99
ATOM C	2241	С	ALA	A	413	52.735	52.638	8.956	1.00	65.55
MOTA	2242	0	ALA	A	413	52.051	51.614	8.999	1.00	65.26
O ATOM C	2243	СВ	ALA	Α	413	55.212	52.736	8.712	1.00	64.03
ATOM N	2244	N	ARG	A	414	52.53.3	53.676	9.764	1.00	67.81
ATOM	2245	CA	ARG	A	414	51.489	53.671	10.789	1.00	69.46
C · ATOM C	2246	С	ARG	A	414	50.087	53.325	10.285	1.00	70.36
ATOM O	2247	0	ARG	A	414	49.181	53.071	11.084	1.00	70.13
MOTA	2248	СВ	ARG	Α	414	51.446	55.026	11.509	1.00	70.05
C ATOM	2249	CG	ARG	Α	414	50.960	56.194	10.659	1.00	71.62
C ATOM C	2250	CD	ARG	A	414	50.711	57.418	11.534	1.00	73.27
ATOM N	2251	NE	ARG	A	414	50.149	58.551	10.799	1.00	74.95
MOTA	2252	CZ	ARG	A	414	50.825	59.302	9.933	1.00	75.82
C ATOM N	2253	NH1	ARG	A	414	52.102	59.047	9.682	1.00	76.36
ATOM N	2254	NH2	ARG	A	414	50.225	60.317	9.323	1.00	76.47
ATOM	2255	N	ASŅ	A	415	49.911	53.313	8.967	1.00	71.18
N ATOM C	2256	CA	ASN	A	415 .	48.617	53.001	8.364	1.00	72.52
ATOM C	2257	C	ASN	A	415	48.712	51.666	7.617	1.00	73.18
MOTA	2258	0	ASN	A	415	48.989	51.638	6.416	1.00	73.46
O ATOM C	2259	СВ	ASN	A	415	48.218	54.124	7.393	1.00	73.28
ATOM C	2260	CG	ASN	A	415	46.759	54.059	6.982	1.00	73.50
MOTA	2261	OD1	ASN	Α	415	46.348	54.689	5.987	1.00	73.39
O ATOM	2262	ND2	. ASN	Α	415	45.957	53.314	7.742	1.00	73.08
N ATOM N	2263	N	TRP	Α	416	48.482	50.563	8.329	1.00	73.62
ATOM C	2264	CA	TRP	Α	416	48.564	49.238	7.716	1.00	74.23

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ATOM C	2265	С	TRP	A	416	47.212	48.527	7.660	1.00	73.85
ATOM O	2266	0	TRP	A	416	46.416	48.598	8.598	1.00	73.60
ATOM C	2267	CB	TRP	A	416	49.593	48.374	8.468	1.00	74.70
ATOM C	2268	CG	TRP	A	416	49.043	47.556	9.609	1.00	76.10
ATOM C	2269	CD1	TRP	A	416	48.308	46.405	9.516	1.00	76.57
ATOM C	2270	CD2	TRP	A	416	49.195	47.819	11.010	1.00	76.67
ATOM N	2271	NE1	TRP	A	416	47.996	45.936	10.770	1.00	76.56
ATOM C	2272	CE2	TRP	A	416	48.527	46.784	11.705	1.00	76.89
ATOM C	2273	CE3	TRP	A	416	49.830	48.828	11.747	1.00	77.37
ATOM C	2274	CZ2	TRP	A	416	48.477	46.729	13.102	1.00	77.40
ATOM C	2275	CZ3	TRP	A	416	49.780	48.772	13.138	1.00	77.75
ATOM C	2276	CH2	TRP	A	416	49.107	47.728	13.799	1.00	77.84
ATOM	2277	N	GLU	A	431	54.545	62.823	11.142	1.00	66.75
N ATOM C	2278	CA	GLU	A	431	54.941	62.244	12.421	1.00	66.57
ATOM C	2279	С	GLU	A	431	56.245	61.460	12.283	1.00	65.93
ATOM	2280	0	GĻU	A	431	56.929	61.185	13.270	1.00	66.27
O ATOM C	2281	СВ	GLU	A	431	53.832	61.328	12.945	1.00	67.44
ATOM C	2282	CG	GLU	A	431	52.495	62.032	13.143	1.00	68.98
ATOM C	2283	CD	GLU	A	431	51.422	61.112	13.693	1.00	69.90
ATOM O	2284	OE1	GLU	A	431	51.073	60.126	13.010	1.00	70.49
ATOM O	2285	OE2	GLU	A	431	50.927	61.373	14.811	1.00	70.56
ATOM	2286	N	GLY	A	432	56.582	61.106	11.047	1.00	64.87
N ATOM C	2287	CA	GLY	A	432	57.803	60.367	10.786	1.00	63.17
ATOM C	2288	С	GLY	A	432	58.332	60.728	9.414	1.00	62.04
ATOM	2289	0	GLY	A	432	57.658	61.423	8.654	1.00	62.22
O ATOM	2290	N	VAL	A	433	59.533	60.262	9.085	1.00	60.59
N ATOM	2291	CA	VAL	A	433	60.117	60.564	7.785	1.00	58.60
C ATOM C	2292	С	VAL	Α	433	60.530	59.318	7.000	1.00	57.08

ATOM O	2293	0	VAL	A	433	60.849	58.276	7.576	1.00	56.04
ATOM C	2294	СВ	VAL	A	433	61.336	61.508	7.930	1.00	58.79
MOTA	2295	CG1	VAL	A	433	60.883	62.858	8.459	1.00	58.84
C ATOM C	2296	CG2	VAL	A	433	62.359	60.901	8.867	1.00	58.98
ATOM N	2297	N	ASP	A	434	60.507	59.446	5.676	1.00	55.12
ATOM	2298	CA	ASP	A	434	60.867	58.367	4.761	1.00	53.00
C ATOM C	2299	С	ASP	A	434	62.215	58.734	4.144	1.00	51.90
ATOM O	2300	0	ASP	A	434	62.401	59.866	3.696	1.00	51.71
ATOM	2301	CB	ASP	A	434	59.799	58.250	3.667	1.00	53.31
C ATOM C	2302	CG	ASP	A	434	59.932	56.984	2.841	1.00	53.22
ATOM	2303	OD1	ASP	A	434	59.210	56.862	1.830	1.00	53.79
O ATOM O	2304	OD2	ASP	A	434	60.744	56.108	3.199	1.00	53.37
MOTA	2305	N	SER	A	435	63.153	57.792	4.106	1.00	50.14
N ATOM C	2306	CA	SER	A	435	64.471	58.098	3.560	1.00	48.49
ATOM	2307	C	SER	A	435	65.267	56.912	3.026	1.00	47.19
C ATOM	2308	0	SER	A	435	64.748	55.809	2.862	1.00	46.05
O ATOM C	2309	СВ	SER	A	435	65.304	58.806	4.627	1.00	48.72
ATOM O	2310	OG	SER	A	435	65.451	57.976	5.768	1.00	49.51
ATOM N	2311	N	TYR	A	436	66.545	57.169	2.765	1.00	46.20
ATOM C	2312	CA	TYR	A	436	67.470	56.163	2.259	1.00	46.22
ATOM C	2313	С	TYR	A	436	68.735	56.149	3.114	1.00	45.31
MOTA	2314	0	TYR	A	436	69.125	57.175	3.673	1.00	45.33
O ATOM C	2315	СВ	TYR	A	436	67.858	56.481	0.812	1.00	48.04
ATOM C	2316	CG	TYR	A	436	66.731	56.356	-0.186	1.00	49.05
ATOM	2317	CD1	TYR	A	436	66.236	55.106	-0.555	1.00	49.71
C ATOM C	2318	CD2	TYR	. A	436	66.160	57.488	-0.764	1.00	50.33
ATOM C	2319	CE1	TYR	. A	436	65.198	54.987	-1.476	1.00	50.76
ATOM C	2320	CE2	TYR	A	436	65.119	57.381	-1.685	1.00	50.87

ATOM C	2321	CZ	TYR	A	436	64.645	56.129	-2.035	1.00	50.97
ATOM O	2322	ОН	TYR	A	436	63.614	56.019	-2.940	1.00	52.36
MOTA	2323	N	VAL	A	437	69.361	54.980	3.217	1.00	44.07
N ATOM C	2324	CA	VAL	A	437	70.602	54.824	3.970	1.00	43.32
ATOM C	2325	С	VAL	A	437	71.591	54.068	3.092	1.00	42.81
ATOM	2326	0	VAL	A	437	71.218	53.132	2.384	1.00	41.76
O ATOM C	2327	CB	VAL	A	437	70.401	54.034	5.290	1.00	42.99
ATOM C	2328	CG1	VAĻ	A	437	69.463	54.793	6.213	1.00	42.96
ATOM C	2329	CG2	VAL	À	437	69.868	52.645	4.997	1.00	42.44
ATOM N	2330	N	PRO	A	438	72.873	54.460	3.133.	1.00	43.06
ATOM C	2331	CA	PRO	A	438	73.882	53.784	2.313	1.00	42.54
ATOM	2332	С	PRO	A	438	73.998	52.295	2.611	1.00	41.85
C ATOM O	2333	0	PRO	A	438	74.038	51.883	3.770	1.00	41.55
ATOM C	2334	ĊB	PRO	A	438	75.162	54.554	2.641	1.00	43.10
ATOM	2335	CG	PRO	A	438	74.943	54.958	4.067	1.00	44.10
C ATOM C	2336	CD	PRO	A	438	73.501	55.422	4.056	1.00	42.97
ATOM N	2337	N	TYR	A	439	74.034	51.491	1.554	1.00	41.03
ATOM C	2338	CA	TYR	A	439	74.162	50.046	1.686	1.00	40.53
ATOM C	2339	С	TYR	A	439	75.502	49.754	2.356	1.00	40.67
ATOM O	2340-	0	TYR	A	439	76.530	50.308	1,.968	1.00	39.93
ATOM C	2341	СВ	TYR	A	439	74.108	49.393	0.303	1.00	40.18
	2342	CG	TYR	A	439	74.244	47.889	0.305	1.00	39.32
ATOM C	2343	CD1	TYR	A	439	73.339	47.086	0.998	1.00	40.13
ATOM C	2344	CD2	TYR	A	439	75.264	47.263	-0.411	1.00	39.93
ATOM C	2345	CE1	TYR	A	439	73.445	45.697	0.975	1.00	40.31
ATOM C	2346	CE2	TYR	A	439	75.380	45.878	-0.439	1.00	39.98
ATOM C	2347	CZ	TYR	A	439	74.467	45.102	0.254	1.00	40.61
ATOM O	2348	ОН	TYR	A	439	74.576	43.731	0.226	1.00	41.51

ATOM N	2349	N	ALA	A	440	75.485	48.885	3.361	1.00	40.76
ATOM C	2350	CA	ALA	A	440	76.699	48.546	4.091	1.00	41.53
ATOM C	2351	С	ALA	A	440	77.102	47.093	3.899	1.00	41.13
ATOM O	2352	0	ALA	A	440	78.175	46.679	4.330	1.00	41.96
ATOM C	2353	СВ	ALA	A	440	76.507	48.842	5.580	1.00	40.70
ATOM N	2354	N	GLY	A	441	76.239	46.320	3.251	1.00	41.41
ATOM C	2355	CA	GLY	A	441	76.536	44.919	3.030	1.00	41.21
ATOM C	2356	С	GLY	Α	441	75.917	44.025	4.088	1.00	41.44
ATOM O	2357	0	GLY	A	441	74.882	44.359	4.664	1.00	41.15
ATOM N	2358	N .	LYS	A	442	76.562	42.891	4.345	1.00	41.60
ATOM C	2359	CA	LYS	A	442	76.097	41.917	5.329	1.00	41.97
ATOM C	2360	С	LYS	A	442	76.237	42.410	6.771	1.00	40.70
ATOM O	2361	0	LYS	A	442	77.189	43.112	7.114	1.00	41.12
ATOM C	2362	СВ	LYS	A	442	76.880	40.613	5.168	1.00	43.78
ATOM C	2363	CG	LYS	A	442	76.859	40.049	3.756	1.00	46.44
ATOM C	2364	CD	LYS	A	442	75.487	39.510	3.386	1.00	47.81
ATOM C	2365	CE	LYS	A	442	75.159	38.260	4.179	1.00	48.88
ATOM N	2366	NZ	LYS	A	442	73.844	37.682	3.783	1:00	51.00
ATOM N	2367	N	LEU	A	443	75.285	42.020	7.611	1.00	39.20
ATOM C	2368	CA	LEU	A	443	75,280	42.405	9.021	1.00	36.87
ATOM C	2369	С	LEU	A	443	76.534	41.935	9.758	1.00	36.82
ATOM O	2370	0	LEU	A	443	77.190	42.715	10.451	1.00	34.89
ATOM C	2371	СВ	LEU	A	443	74.032	41.829	9.703	1.00	35.37
ATOM C	2372	CG	LEU	A	443	73.831	42.033	11.210	1.00	34.30
ATOM C	2373	CD1	LEU	A	443	72.354	41.880	11.554	1.00	34.00
ATOM C	2374	CD2	LEU	A	443	74.673	41.028	11.990	1.00	33.34
MOTA	2375	N	LYS	A	444	76.864	40.660	9.593	1.00	36.78
N ATOM C	2376	CA	LYS	A	444	78.016	40.052	10.256	1.00	37.95

ATOM C	2377	C	LYS	A	444	79.303	40.880	10.292	1.00	37.79
ATOM O	2378	0 .	LYS	Α	444	79.801	41.211	11.371	1.00	36.54
ATOM	2379	СВ	LYS	Α	444	78.318	38.687	9`.629	1.00	39.41
C ATOM C	2380	CG	LYS	A	444	79.374	37.896	10.380	1.00	43.18
ATOM C	2381	CD	LYS	A	444	79.656	36.560	9.716	1.00	45.77
ATOM C	2382	CE	LYS	A	444	80.661	35.762	10.527	1.00	47.73
ATOM N	2383	NZ	LYS	A	444	81.910	36.539	10.764	1.00	49.70
ATOM N	2384	N	ASP	Α	445	79.839	41.207	9.120	1.00	37.04
ATOM C	2385	CA	ASP	A	445	81.086	41.965	9.023	1.00	37.29
ATOM C	2386	С	ASP	A	445	81.040	43.353	9.645	1.00	35.93
ATOM O	2387	0	ASP	A	445	82.032	43.819	10.208	1.00	34.89
ATOM C	2388	CB	ASP	A	445	81.512	42.095	7.558	1.00	39.90
MOTA	2389	CG	ASP	A	445	81.673	40.750	6.876	1.00	42.77
C ATOM O	2390	OD1	ASP	A	445	82.442	39.906	7.389	1.00	43.80
ATOM O	2391	OD2	ASP	A	445	81.025	40.541	5.827	1.00	45.60
ATOM N	2392	N	ASN	A	446	79.897	44.020	9.525	1.00	33.98
ATOM C	2393	CA	ASN	A	446	79.739	45.359	10.075	1.00	33.10
ATOM C	2394	С	ASN	A	446	79.657	45.330	11.596	1.00	31.88
ATOM O	2395	0	ASN	A	446	80.257	46.167	12.272	1.00	30.91
MOTA	2396	СВ	ASN	A	446	78.489	46.016	9.493	1.00	33.95
C ATOM C	2397	CG	ASN	A	446	78.683	46.454	8.051	1.00	35.61
ATOM	2398	OD1	ASN	A	446	79.267	47.505	7.785	1.00	37.12
O ATOM	2399	ND2	ASN	A	446	78.207	45.641	7.116	1.00	34.41
N ATOM N	2400	N	VAL	A	447	78.911	44.371	12.131	1.00	31.04
ATOM C	2401	CA	VAL	A	447	78.776	44.244	13.576	1.00	31.31
ATOM	2402	С	VAL	A	447	80.130	43.896	14.195	1.00	32.24
C ATOM O	2403	0	VAL	A	447	80.503	44.444	15.228	1.00	32.11
ATOM C	2404	CB	VAL	A	447	77.740	43.160	13.949	1.00	30.45

ATOM C	2405	CG1	VAL	A	447	77.813	42.858	15.443	1.00	30.61
ATOM C	2406	CG2	VAL	A	447	76.336	43.642	13.587	1.00	30.05
ATOM N	2407	N	GLU	A	448	80.863	42.988	13.559	1.00	32.57
ATOM C	2408	CA	GLU	A	448	82.178	42.594	14.061	1.00	33.80
ATOM C	2409	С	GLU	A	448	83.095	43.819	14.130	1.00	32.73
ATOM O	2410	0	GLU	A	448	83.794	44.029	15.125	1.00	31.37
ATOM C	2411	CB	GLU	A	448	82.798	41.529	13.148	1.00	37.00
ATOM C	2412	CG	GLU	A	448	84.116	40.945	13.658	1.00	41.15
ATOM C	2413	CD	GLU	A	448	84.710	39.904	12.714	1.00	44.90
ATOM O	2414	OE1	GLU	A	448	85.161	40.280	11.610	1.00	47.11
ATOM O	2415	OE2	GLU	A	448	84.720	38.705	13.075	1,00	47.09
ATOM N	2416	N	ALA	Ä	449	83.086	44.630	13.076	1.00	31.13
ATOM C	2417	CA	ALA	A	449	83.918	45.829	13.034	1.00	31.18
ATOM C	2418	С	ALA	A	449	83.528	46.810	14.137	1.00	30.71
ATOM O	2419	0	ALA	A	449	84.385	47.323	14.854	1.00	29.77
ATOM C	2420	CB	ALA	A	449	83.802	46.506	11.674	1.00	31.83
ATOM N	2421	N	SER	A	450	82.232	47.068	14.269	1.00	29.54
ATOM C	2422	CA	SER	A	450	81.747	47.990	15.289	1.00	30.17
ATOM C	2423	С	SER	A	450	82.130	47.528	16.694	1.00	30.40
ATOM O	2424	0	SER	A	450	82.690	48.298	17.477	1.00	29.79
ATOM .	2425	CB	SER	A	450	80.220	48.126	15.208	1.00	29.18
ATOM O	2426	OG	SER	A	450	79.822	48.804	14.031	1.00	29.75
ATOM N	2427	N	LEU	A	451	81.832	46.269	17.006	1.00	29.78
ATOM C	2428	CA	LEU	A	451	82.123	45.734	18.330	1.00	30.57
ATOM C	2429	С	LEU	A	451	83.614	45.586	18.620	1.00	31.46
ATOM O	2430	0	LEU	A	451	84.022	45.603	19.781	1.00	30.55
ATOM C	2431	СВ	LEU	Α	451	81.389	44.406	18.538	1.00	30.40
ATOM C	2432	CG	LEU	A	451	79.858	44.540	18.505	1.00	30.16

2433	CD1	LEU	A	451	79.219	43.219	18.883	1.00	30.36
2434	CD2	LEU	A	451	79.409	45.640	19.466	1.00	30.38
2435	N	ASN	A	452	84.430	45.440	17.580	1.00	32.01
2436	CA	ASN	A	452	85.869	45.344	17.800	1.00	33.62
2437	C .	ASN	A	452	86.349	46.699	18.319	1.00	33.02
2438	0	ASN	Α	452	87.226	46.771	19.181	1.00	32.70
2439	CB	ASN	A	452	86.615	44.988	16.510	1.00	35.58
2440	CG	ASN	A	452	86.569	43.505	16.201	1.00	39.03
2441	OD1	ASN	A	452	86.531	42.669	17.109	1.00	41.67
2442	ND2	ASN	A	452	86.595	43.167	14.916	1.00	41.46
2443	N	LYS	A	453	85.761	47.772	17.795	1.00	32.33
2444	CA	LYS	A	453	86,125	49.115	18.225	1.00	32.17
2445	С	LYS	A	453	85.642	49.343	19.655	1.00	30.92
2446	0	LYS	A	453	86.344	49.949	20.459	1.00	29.86
2447	CB	LYS	A	453	85.528	50.161	17.278	1.00	33.56
2448	CG	LYS	A	453	86.172	50.131	15.889	1,00	37.25
2449	CD	LYS	A	453	85.461	51.033	14.892	1.00	37.79
2450	CE	LYS	A	453	85.502	52.490	15.316	1.00	39.41
2451	NZ	LYS	A	453	84.804	53.342	14.314	1.00	40.64
2452	N	VAL	A	454	84.447	48.849	19.966	1.00	29.21
2453	CA	VAL	Α	454	83.900	48.981	21.311	1.00	28.29
2454	C	VAL	A	454	84.827	48.253	22.290	1.00	29.16
2455	0	VAL	A	454	85.196	48.801	23.330	1.00	27.96
2456	СВ	VAL	A	454	82.478	48.368	21.408	1.00	28.44
2457	CG1	VAL	A	454	82.016	48.334	22.867	1.00	26.28
2458	CG2	VAL	A	454	81.499	49.188	20.571	1.00	27.61
2459	N	LYS	A	455	85.209	47.024	21.945	1.00	28.54
2460	CA	LYS	A	455	86.092	46.229	22.801	1.00	29.86
	2434 2435 2436 2437 2438 2439 2440 2441 2442 2443 2445 2446 2447 2448 2449 2450 2451 2452 2453 2454 2455 2456 2457 2458	2434 CD2 2435 N 2436 CA 2437 C 2438 O 2439 CB 2440 CG 2441 OD1 2442 ND2 2443 N 2444 CA 2445 C 2446 O 2447 CB 2448 CG 2449 CD 2450 CE 2451 NZ 2452 N 2452 N 2453 CA 2455 O 2456 CB 2457 CG1 2458 CG2 2459 N	2434       CD2       LEU         2435       N       ASN         2436       CA       ASN         2438       O       ASN         24439       CB       ASN         2441       OD1       ASN         2442       ND2       ASN         2443       N       LYS         2444       CA       LYS         2446       O       LYS         2447       CB       LYS         2449       CD       LYS         2450       CE       LYS         2451       NZ       LYS         2452       N       VAL         2453       CA       VAL         2455       O       VAL         2456       CB       VAL         2457       CG1       VAL         2458       CG2       VAL         2459       N       LYS	24334       CD2       LEU       A         2435       N       ASN       A         2436       CA       ASN       A         2437       C       ASN       A         2439       CB       ASN       A         2440       CG       ASN       A         2441       OD1       ASN       A         2442       ND2       ASN       A         2443       N       LYS       A         2444       CA       LYS       A         2446       O       LYS       A         2447       CB       LYS       A         2449       CD       LYS       A         2450       CE       LYS       A         2451       NZ       LYS       A         2452       N       VAL       A         2453       CA       VAL       A         2454       C       VAL       A         2455       O       VAL       A         2456       CB       VAL       A         2456       CB       VAL       A         2458       CG       VAL       A	24334       CD2       LEU       A       451         24355       N       ASN       A       452         2436       CA       ASN       A       452         2437       C       ASN       A       452         2438       O       ASN       A       452         2449       CB       ASN       A       452         2440       CG       ASN       A       452         2441       OD1       ASN       A       452         2442       ND2       ASN       A       452         2443       N       LYS       A       453         2444       CA       LYS       A       453         2444       CA       LYS       A       453         2444       CA       LYS       A       453         2446       O       LYS       A       453         2447       CB       LYS       A       453         2448       CG       LYS       A       453         2459       CE       LYS       A       453         2451       NZ       LYS       A       453 <td< td=""><td>2434       CD2       LEU A 451       79.409         2435       N       ASN A 452       84.430         2436       CA       ASN A 452       85.869         2437       C       ASN A 452       86.349         2438       O       ASN A 452       86.615         2440       CG       ASN A 452       86.615         2440       CG       ASN A 452       86.569         2441       OD1       ASN A 452       86.595         2442       ND2       ASN A 452       86.595         2443       N       LYS A 453       85.761         2444       CA       LYS A 453       85.761         2444       CA       LYS A 453       85.642         2445       C       LYS A 453       85.528         2446       O       LYS A 453       85.528         2447       CB       LYS A 453       85.528         2448       CG       LYS A 453       85.528         2449       CD       LYS A 453       85.502         2451       NZ       LYS A 453       85.502         2451       NZ       LYS A 453       85.502         2451       NZ       LYS</td><td>2434       CD2       LEU A 451       79.409       45.640         2435       N       ASN A 452       84.430       45.440         2436       CA       ASN A 452       85.869       45.344         2437       C       ASN A 452       86.349       46.699         2438       O       ASN A 452       87.226       46.771         2439       CB       ASN A 452       86.615       44.988         2440       CG       ASN A 452       86.569       43.505         2441       OD1       ASN A 452       86.569       43.167         2442       ND2       ASN A 452       86.595       43.167         2443       N       LYS A 453       85.761       47.772         2444       CA       LYS A 453       86.125       49.115         2444       CA       LYS A 453       86.344       49.949         2445       C       LYS A 453       86.344       49.949         2446       O       LYS A 453       86.125       50.161         2447       CB       LYS A 453       86.172       50.131         2449       CD       LYS A 453       85.502       52.490         24</td><td>2434 CD2 LEU A 451 79.409 45.640 19.466 2435 N ASN A 452 84.430 45.440 17.580 2436 CA ASN A 452 85.869 45.344 17.800 2437 C ASN A 452 86.349 46.699 18.319 2438 O ASN A 452 86.615 44.988 16.510 2440 CG ASN A 452 86.569 43.505 16.201 2441 OD1 ASN A 452 86.569 43.505 16.201 2442 ND2 ASN A 452 86.595 43.167 14.916 2443 N LYS A 453 85.761 47.772 17.795 2444 CA LYS A 453 85.642 49.343 19.655 2446 O LYS A 453 85.642 49.343 19.655 2446 O LYS A 453 85.642 49.949 20.459 2447 CB LYS A 453 85.528 50.161 17.278 2448 CG LYS A 453 85.461 51.033 14.892 2449 CD LYS A 453 85.461 51.033 14.892 2450 CE LYS A 453 85.461 51.033 14.892 2451 NZ LYS A 453 85.461 51.033 14.892 2452 N VAL A 454 84.804 53.342 14.314 2452 N VAL A 454 84.804 53.342 14.314 2454 C VAL A 454 84.847 48.849 19.966 2453 CA VAL A 454 84.827 48.253 22.290 2456 CB VAL A 454 82.478 48.368 21.408 2457 CG1 VAL A 454 82.478 48.368 21.408 2458 CG2 VAL A 454 82.478 48.368 21.408 2459 CG1 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408 2459 CG1 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408</td><td>2434 CD2 LEU A 451 79.409 45.640 19.466 1.00 2435 N ASN A 452 84.430 45.440 17.580 1.00 2436 CA ASN A 452 86.349 46.699 18.319 1.00 2438 O ASN A 452 86.349 46.699 18.319 1.00 2439 CB ASN A 452 86.615 44.988 16.510 1.00 2440 CG ASN A 452 86.569 43.505 16.201 1.00 2441 OD1 ASN A 452 86.595 43.167 14.916 1.00 2442 ND2 ASN A 452 86.595 43.167 14.916 1.00 2443 N LYS A 453 85.761 47.772 17.795 1.00 2444 CA LYS A 453 85.642 49.343 19.655 1.00 2445 C LYS A 453 86.344 49.949 20.459 1.00 2446 CB LYS A 453 86.344 49.949 20.459 1.00 2447 CB LYS A 453 86.344 49.949 20.459 1.00 2448 CG LYS A 453 86.172 50.131 15.889 1.00 2449 CD LYS A 453 85.642 50.161 17.278 1.00 2449 CD LYS A 453 85.461 51.033 14.892 1.00 2450 CE LYS A 453 85.461 51.033 14.892 1.00 2451 NZ LYS A 453 84.804 53.342 14.314 1.00 2452 N VAL A 454 84.804 53.342 14.314 1.00 2453 CA VAL A 454 84.847 48.849 19.966 1.00 2455 CB VAL A 454 84.827 48.253 22.290 1.00 2456 CB VAL A 454 84.827 48.253 22.290 1.00 2457 CG1 VAL A 454 82.478 48.334 22.867 1.00 2458 CG2 VAL A 454 82.478 48.334 22.867 1.00 2458 CG2 VAL A 454 82.478 48.334 22.867 1.00 2459 N LYS A 453 85.209 47.024 21.945 1.00</td></td<>	2434       CD2       LEU A 451       79.409         2435       N       ASN A 452       84.430         2436       CA       ASN A 452       85.869         2437       C       ASN A 452       86.349         2438       O       ASN A 452       86.615         2440       CG       ASN A 452       86.615         2440       CG       ASN A 452       86.569         2441       OD1       ASN A 452       86.595         2442       ND2       ASN A 452       86.595         2443       N       LYS A 453       85.761         2444       CA       LYS A 453       85.761         2444       CA       LYS A 453       85.642         2445       C       LYS A 453       85.528         2446       O       LYS A 453       85.528         2447       CB       LYS A 453       85.528         2448       CG       LYS A 453       85.528         2449       CD       LYS A 453       85.502         2451       NZ       LYS A 453       85.502         2451       NZ       LYS A 453       85.502         2451       NZ       LYS	2434       CD2       LEU A 451       79.409       45.640         2435       N       ASN A 452       84.430       45.440         2436       CA       ASN A 452       85.869       45.344         2437       C       ASN A 452       86.349       46.699         2438       O       ASN A 452       87.226       46.771         2439       CB       ASN A 452       86.615       44.988         2440       CG       ASN A 452       86.569       43.505         2441       OD1       ASN A 452       86.569       43.167         2442       ND2       ASN A 452       86.595       43.167         2443       N       LYS A 453       85.761       47.772         2444       CA       LYS A 453       86.125       49.115         2444       CA       LYS A 453       86.344       49.949         2445       C       LYS A 453       86.344       49.949         2446       O       LYS A 453       86.125       50.161         2447       CB       LYS A 453       86.172       50.131         2449       CD       LYS A 453       85.502       52.490         24	2434 CD2 LEU A 451 79.409 45.640 19.466 2435 N ASN A 452 84.430 45.440 17.580 2436 CA ASN A 452 85.869 45.344 17.800 2437 C ASN A 452 86.349 46.699 18.319 2438 O ASN A 452 86.615 44.988 16.510 2440 CG ASN A 452 86.569 43.505 16.201 2441 OD1 ASN A 452 86.569 43.505 16.201 2442 ND2 ASN A 452 86.595 43.167 14.916 2443 N LYS A 453 85.761 47.772 17.795 2444 CA LYS A 453 85.642 49.343 19.655 2446 O LYS A 453 85.642 49.343 19.655 2446 O LYS A 453 85.642 49.949 20.459 2447 CB LYS A 453 85.528 50.161 17.278 2448 CG LYS A 453 85.461 51.033 14.892 2449 CD LYS A 453 85.461 51.033 14.892 2450 CE LYS A 453 85.461 51.033 14.892 2451 NZ LYS A 453 85.461 51.033 14.892 2452 N VAL A 454 84.804 53.342 14.314 2452 N VAL A 454 84.804 53.342 14.314 2454 C VAL A 454 84.847 48.849 19.966 2453 CA VAL A 454 84.827 48.253 22.290 2456 CB VAL A 454 82.478 48.368 21.408 2457 CG1 VAL A 454 82.478 48.368 21.408 2458 CG2 VAL A 454 82.478 48.368 21.408 2459 CG1 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408 2459 CG1 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408 2459 CG2 VAL A 454 82.478 48.368 21.408	2434 CD2 LEU A 451 79.409 45.640 19.466 1.00 2435 N ASN A 452 84.430 45.440 17.580 1.00 2436 CA ASN A 452 86.349 46.699 18.319 1.00 2438 O ASN A 452 86.349 46.699 18.319 1.00 2439 CB ASN A 452 86.615 44.988 16.510 1.00 2440 CG ASN A 452 86.569 43.505 16.201 1.00 2441 OD1 ASN A 452 86.595 43.167 14.916 1.00 2442 ND2 ASN A 452 86.595 43.167 14.916 1.00 2443 N LYS A 453 85.761 47.772 17.795 1.00 2444 CA LYS A 453 85.642 49.343 19.655 1.00 2445 C LYS A 453 86.344 49.949 20.459 1.00 2446 CB LYS A 453 86.344 49.949 20.459 1.00 2447 CB LYS A 453 86.344 49.949 20.459 1.00 2448 CG LYS A 453 86.172 50.131 15.889 1.00 2449 CD LYS A 453 85.642 50.161 17.278 1.00 2449 CD LYS A 453 85.461 51.033 14.892 1.00 2450 CE LYS A 453 85.461 51.033 14.892 1.00 2451 NZ LYS A 453 84.804 53.342 14.314 1.00 2452 N VAL A 454 84.804 53.342 14.314 1.00 2453 CA VAL A 454 84.847 48.849 19.966 1.00 2455 CB VAL A 454 84.827 48.253 22.290 1.00 2456 CB VAL A 454 84.827 48.253 22.290 1.00 2457 CG1 VAL A 454 82.478 48.334 22.867 1.00 2458 CG2 VAL A 454 82.478 48.334 22.867 1.00 2458 CG2 VAL A 454 82.478 48.334 22.867 1.00 2459 N LYS A 453 85.209 47.024 21.945 1.00

ATOM C	2461	.C	LYS A	455	87.443	46.901	23.011	1.00 29.20
ATOM O	2462	0	LYS A	455	87.990	46.887	24.114	1.00 28.77
ATOM C	2463	СВ	LYS A	455	86.322	44.838	22.202	1.00 30.13
ATOM C	2464	CG	LYS A	455	85.109	43.927	22.179	1.00 32.41
ATOM C	2465	CD	LYS F	455	85.465	42.639	21.447	1.00 34.53
ATOM C	2466	CE	LYS A	455	84.273	41.723	21.273	1.00 37.13
ATOM N	2467	NZ	LYS A	455	84.641	40.530	20.457	1.00 38.19
ATOM N	2468	N	SER A	456	87.985	47.483	21.946	1.00 29.06
ATOM C	2469	CA	SER A	456	89.271	48.152	22.036	1.00 30.21
ATOM C	2470	С	SER A	456	89.173	49.345	22.988	1.00, 29.49
ATOM O	2471	0	SER A	456	90.051	49.565	23.823	1.00 28.06
ATOM C	2472	CB	SER A	A 456	89.722	`48.617	20.650	1.00 31.84
ATOM O	2473	OG	SER A	A 456.	91.050	49.100	20.703	1.00 36.19
ATOM N	2474	N .	THR A	457	88.090	50.106	22.863	1.00 27.42
ATOM C	-2475	CA	THR A	A 457	87.872	51.265	23.717	1.00 27.12
ATOM C	2476	С	THR A	A 457	87.689	50.822	25.163	1.00 26.61
ATOM O	2477	0	THR A	A 457	88.174	51.476	26.087	1.00 26.73
ATOM C	2478	CB	THR A	A 457	86.636	52.051	23.254	1.00 27.39
ATOM O	2479	OG1	THR A	457	86.833	52.456	21.897	1.00 29.71
ATOM C	2480	CG2	THR A	A 457	86.416	53.278	24.121	1.00 25.69.
ATOM N	2481	N	MET A	458	86.993	49.706	25.362	1.00 25.76
ATOM C	2482	CA	MET A	A 458	86.791	49.197	26.708	1.00 25.74
ATOM C	2483	С	MET A	458	88.145	48.903	27.349	1.00 26.35
ATOM O	2484	o	MET A	458	88.373	49.229	28.518	1.00 24.96
ATOM C	2485	CB	MET A	A 458	85.900	47.954	26.670	1.00 25.80
ATOM C	2486	CG	MET 2	A 458	84.427	48.318	26.457	1.00 25.05
ATOM S	2487	SD	MET A	A 458	83.363	46.907	26.197	1.00 26.75
ATOM C	2488	CE	MET 2	A 458	83.422	46.109	27.816	1.00 25.98

ATOM N	2489	N	CYS	A	459	89.061	48.320	26.582	1.00	26.5 <b>4</b>
ATOM C	2490	CA	CYS	A	459	90.388	48.043	27.124	1.00	28.58
ATOM C	2491	C	CYS	A	459	91.144	49.331	27.465	1.00	27.83
ATOM O	2492	0	CYS	Α	459	91.932	49.357	28.414	1.00	27.16
ATOM C	2493	CB	CYS	A	459	91.201	47.183	26.159	1.00	31.43
ATOM S	2494	SG	CYS	A	459	90.785	45.417	26.328	1.00	37.59
ATOM N	2495	N	ASN	Α	460	90.913	50.393	26.696	1.00	27.31
ATOM C	2496	CA	ASN	A	460	91.554	51.678	26.978	1.00	26.88
ATOM C	2497	С	ASN	A	460	91.053	52.139	28.347	1.00	27.10
ATOM O	2498	0	ASN	À	460	91.792	52.748	29.122	1.00	25.93
ATOM .	2499	CB	ASN	A	460	91.168	52.744	25.942	1.00	27.20
ATOM C	2500	CG	ASN	A	460	91.839	52.542	24.595	1.00	30.02
ATOM O	2501	OD1	ASN	A	460	91.164	52.420	23.572	1.00	29.71
ATOM N	2502	ND2	ASN	A	460	93.170	52.524	24.583	1.00	29.98
ATOM N	2503	N	CYS	A	461	89.786	51.847	28.631	1.00	26.43
ATOM C	2504	CA	CYS	A	461	89.162	52.233	29.891	1.00	26.78
ATOM C	2505	С	CYS	A	461	89.394	51.232	31.024	1.00	26.46
ATOM O	2506	0	CYS	A	461	88.900	51.426	32.134	1.00	27.65
ATOM C	2507	CB	CYS	A	461	87.654	52.436	29.682	1.00	26.90
ATOM S	2508	SG	CYS	A	461	87,253	53.712	28.445	1.00.	29.55
ATOM N	2509	N	GLY-	A	462	90.139	50.168	30.739	1.00	26.72
ATOM C	2510	CA	GLY	A	462	90.430	49.155	31.745	1.00	28.25
ATOM C	2511	С	GLY	A	462	89.272	48.226	32.081	1.00	28.51
ATOM O	2512	0	GLY	Α	462	89.174	47.712	33.204	1.00	28.75
ATOM N	2513	N	ALA	A	463	88.405	47.979	31.106	1.00	26.73
ATOM C	2514	CA	ALA	A	463	87.239	47.136	31.335	1.00	26.80
ATOM C	2515	С	ALA	A	463	87.198	45.909	30.435	1.00	27.34
ATOM O	2516	0	ALA	A	463	87.350	46.018	29.218	1.00	27.58

C				••	463	85.967	47.963	31.140	1.00	26.04
ATOM N	2518	N	LEU	A	464	86.983	44.746	31.045	1.00	26.85
ATOM C	2519	CA	LEU	A	464	86.896	43.489	30.308	1.00	27.73
ATOM C	2520	С	LEU	A	464	85.447	43.057	30.121	1.00	26.69
ATOM O	2521	0	LEU	Α	464	85.169	42.119	29.379	1.00	27.47
ATOM C	2522	CB	LEU	A	464	87.654	42.378	31.038	1.00	28.53
ATOM C	2523	CG	LEU	A	464	89.176	42.386	30.902	1.00	31.51
ATOM C	2524	CD1	·LEU	A	464	89.777	41.251	31.734	1.00	32.32
ATOM C	2525	CD2	LEU	A	464	89.545	42.218	29.442	1.00	31.92
ATOM N	2526	N	THR	A	465	84.531	43.734	30.806	1.00	25.40
ATOM C	2527	CA	THR	A	465	83.108	43.421	30.709	1.00	24.59
ATOM C	2528	С	THR	A	465	82.320	44.716	30.749	1.00	24.19
ATOM O	2529	0	THR	A	465	82.855	45.766	31.102	1.00	22.83
ATOM C	2530	СВ	THR	A	465	82.617	42.552	31.884	1.00	24.77
ATOM O	2531	OG1	THR	A	465	82.633	43.331	33.088	1.00	24.88
ATOM C	2532	CG2	THR	A	465	83.507	41.317	32.061	1.00	24.23
ATOM N	2533	N	ILE	A	466	81.040	44.639	30.401	1.00	23.48
ATOM C	2534	CA	ILE	A	466	80.200	45.825	30.410	1.00	22.77
ATOM C	2535	С	ILE	A	466	80.004	46.343	31.839	1.00	23.62
ATOM O	2536	0	ILE	A	466	80.103	47.545	32.082	1.00	22.96
ATOM C	2537	CB	ILE	A	466	78.849	45.538	29.699	1.00	23.94
ATOM C	2538	CG1	ILE	A	466	79.113	45.363	28.194	1.00	22.77
ATOM C	2539	CG2	ILE	A	466	77.856	46.679	29.935	1.00	23.50
ATOM C	2540	CD1	ILE	A	466	77.886	44.941	27.377	1.00	24.77
ATOM N	2541	N	PRO	A	467	79.742	45.448	32.809	1.00	23.36
ATOM C	2542	CA	PRO	A	467	79.563	45.945	34.176	1.00	24.01
ATOM	2543	С	PRO	A	467	80.826	46.648	34.676	1.00	24.80
ATOM O	2544	0	PRO	A	467	80.753	47.640	35.399	1.00	24.96

ATOM C	2545	CB	PRO	A _.	467	79.253	44.676	34.965	1.00	24.77
ATOM C	2546	CG	PRO	A	467	78.516	43.843	33.954	1.00	24.81
ATOM C	2547	CD	PRO	A	467	79.367	44.024	32.720	1.00	23.03
ATOM N	2548	N	GLN	A	468	81.988	46.136	34.287	1.00	25.14
ATOM C	2549	CA	GLN	A	468	83.233	46.754	34.713	1.00	26.45
ATOM C	2550 [,]	С	GLN	A	468	83.394	48.121	34.042	1.00	25.99
ATOM O	2551	0	GLN	A	468	83.909	49.062	34.650	1.00	26.63
ATOM C	2552	СВ	GLN	A	468	84.412	45.829	34.398	1.00	27.40
ATOM C	2553	CG	GLN	A	468	85.759	46.390	34.791	1.00	29.99
ATOM C	2554	CD	GLN	A	468	86.,838	45.328	34.836	1.00	28.82
ATOM O	2555	OE1	GLN	A	468	86.952	44.501	33.934	1.00	27.62
ATOM N	2556	NE2	GLN	A	468	87.648	45.356	35.890	1.00	30.42
ATOM ·	2557	N	LEU	A	469	82.940	48.238	32.796	1.00	24.88
N ATOM C	2558	CA	LEU	Α	469	83.014	49.507	32.081	1.00	24.40
ATOM C	2559	С	LEU	A	469	82.093	50.527	32.753	1.00	24.98
MOTA	2560	0	LEU	A	469	82.447	51.702	32.898	1.00	25.34
O ATOM C	2561	CB	LEU	A	469	82.596	49.332	30.611	1.00	24.62
ATOM C	2562	CG	LEU	A	469	82.396	50.625	29.799	1.00	24.32
ATOM C	2563	CD1	LEU	A	469	83.731	51.286	29.507	1.00	24.10
ATOM	2564	CD2	LEU	A	469	81.681	50.298	28.497	1.00	23.72
ATOM	2565	N	GLN	A	470	80.914	50.077	33.168	1.00	24.91
N ATOM	2566	CA	GLN	A	470	79.951	50.965	33.807	1.00	26.70
C ATOM C	2567	С	GLN	A	470	80.461	51.471	35.151	1.00	27:35
ATOM O	2568	0	GLN	A	470	80.103	52.560	35.601	1.00	28.25
ATOM C	2569	СВ	GLN	A	470	78.614	50.238	33.961	1.00	27.04
ATOM C	2570	CG	GLN	A	470	78.071	49.794	32.600	1.00	26.67
ATOM	2571	CD	GLN	A	470	76.805	48.981	32.688	1.00	27.02
C ATOM O	2572	OE1	GLN	A	470	76.616	48.208	33.621	1.00	28.25
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ATOM N	2573	NE2	GLN	A	470	75.934	49.135	31.696	1.00	25.90
ATOM N	2574	N	SER	A	471	81.316	50.680	35.778	1.00	26.97
ATOM C	2575	CA	SER	A	471	81.883	51.049	37.063	1.00	28.68
ATOM C	2576	С	SER	A	471	83.122	51.944	36.928	1.00	28.52
ATOM O	2577	0	SER	A	471	83.289	52.908	37.680	1.00	29.15
ATOM C	2578	СВ	SER	A	471	82.244	49.775	37.839	1.00	29.10
ATOM O	2579	OG	SER	Α	471	82.934	50.081	39.037	1.00	35.37
ATOM N	2580	N	LYS	A	472	83.968	51.651	35.946	1.00	27.16
ATOM C	2581	CA	LYS	Α	472	85.224	52.390	35.782	1.00	28.51
ATOM C	2582	С	LYS	Ą	472	85.293	53.531	34.778	1.00	27.51
ATOM O	2583	~O	LYS	A	472	86.232	54.323	34.818	1.00	26.25
ATOM C	2584	CB	LYS	A	472	86.341	51.404	35.451	1.00	29.64
ATOM C	2585	CG	LYS	Α	472	86.461	50.273	36.453	1.00	32.63
ATOM C	2586	CD	LYS	A	472	87.440	49.205	35.994	1.00	33.81
ATOM .	258 <b>7</b>	CE	LYS	A	472	88.868	49.704	35.997	1.00	35.59
ATOM N	2588	NZ	LYS	A	472	89.815	48.590	35.715	1.00	35.49
ATOM N	2589	N	ALA	A	473	84.322	53.617	33.876	1.00	26.09
ATOM C	2590	CA	ALA	A	473	84.345	54.660	32.860	1.00	26.12
ATOM C	2591	С	ALA	A	473	84.461	56.080	33.410	1.00	25.21
ATOM O	2592	0	ALA	A	473	83.827	56.432	34.400	1.00	25.99
ATOM C	2593	CB	ALA	A	473	83.106	54.553	31.971	1.00	26.24
ATOM N	2594	N	LYS	A	474	85.290	56.882	32.749	1.00	24.98
ATOM C	2595	CA	LYS	A	474	85.505	58.284	33.098	1.00	25.10
ATOM C	2596	С	LYS	A	474	84.943	59.013	31.884	1.00	24.93
ATOM O	2597	0	LYS	Α	474	85.475	58.904	30.779	1.00	24.89
ATOM C	2598	CB	LYS	A	474	87.000	58.549	33.278	1.00	25.31
	2599	CG	LYS .	A	474	87.589	57.732	34.424	1.00	25.41
	2600	CD	LYS .	A	474	89.078	57.470	34.242	1.00	26.81

ATOM C	2601	CE	LYS	A	474	89.902	58.722	34.425	1.00	28.30
ATOM N	2602	NZ	LYS	A	474	91.346	58.422	34.183	1.00	27.67
ATOM	2603	N	ILE	A	475	83.858	59.750	32.093	1.00	24.28
N ATOM C	2604	CA	ILE	A	475	83.169	60.408	30.986	1.00	25.91
ATOM C	2605	С	ILE	A	475	83.103	61.924	31.100	1.00	25.77
ATOM O	2606	0	ILE	A	475	82.519	62.453	32.042	1.00	26.40
ATOM C	2607	СВ	ILE	A	475	81.726	59.855	30.883	1.00	25.54
ATOM C	2608	CG1	ILE	A	475	81.763	58.319	30.868	1.00	26.29
ATOM	2609	CG2	ILE	A	475	81.043	60.392	29.630	1.00	27.31
C ATOM C	2610	CD1	ILE	A	475	80.394	57.657	30.959	1.00	25.53
ATOM N	2611	N	THR	A	476	83.678	62.617	30.122	1.00	25.85
ATOM	2612	CA	THR	A	476	83.675	64.073	30.140	1.00	25.82
C ATOM C	2613	С	THR	A	476	82.795	64.688	29.067	1.00	25.93
ATOM O	2614	0	THR	Α	476	82.630	64.137	27.977	1.00	24.07
ATOM C	2615	CB	THR	A	476	85.097	64.657	29.955	1.00	26.37
MOTA	2616	OG1	THR	A	476	85.052	66.082	30.123	1.00	28.03
O ATOM C	2617	CG2	THR	A	476	85.625	64.352	28.559	1.00	25.51
ATOM N	2618	N	LEU	A	477	82.232	65.843	29.399	1.00	25.92
ATOM C	2619	CA	LEU	A	477	81.406	66.596	28.472	1.00	27.45
ATOM C	2620	, C	LEU	A	477	82.433	67.442	27.722	1.00	27.85
ATOM O	2621	0	LEU	A	477	83.469	67.780	28.290	1.00	27.59
ATOM	2622	CB	LEU	A	477	80.454	67.501	29.254	1.00	28.30
C ATOM C	2623	CG	LEU	A	477	79.298	68.176	28.523	1.00	30.46
ATOM C	2624	CD1	LEU	A	477	78.351	67.123	27.980	1.00	29.78
ATOM C	2625	CD2	LEU	A	477	78.561	69.099	29.497	1.00	32.80
ATOM N	2626	N	VAL	A	478	82.167	67.771	26.462	1.00	29.07
ATOM C	2627	CA	VAL	A	478	83.095	68.592	25.686	1.00	31.32
ATOM C	2628	С	VAL	A	478	82.456	69.950	25.407	1.00	33.58

ATOM O	2629	0	VAL	Α	478	81.248	70.044	25.212	1.00	32.21
ATOM C	2630	CB	VAL	Α	478	83.480	67.912	24.348	1.00	32.07
ATOM	2631	CG1	VAL	A	478	83.857	66.462	24.604	1.00	32.68
C ATOM C	2632	CG2	VAL	A	478	82.342	68.018	23.341	1.00	34.67
MOTA N	2633	N	SER	Α	479	83.274	70.997	25.385	1.00	35.26
ATOM	2634	CA	SER	A	479	82.791	72.359	25.169	1.00	38.88
C ATOM C	2635	С	SER	A	479	81.991	72.592	23.899	1.00	41.66
ATOM O	2636	0	SER	A	479	82.255	71.993	22.854	1.00	42.05
ATOM	2637	CB	SER	A	479	83.963	73.339	25.174	1.00	38.14
C ATOM O	2638	OG	SER	A	479	84.773	73.130	24.034	1.00	36.16
ATOM N	2639	N	SER	A	480	81.019	73.494	24.004	1.00	45.75
ATOM C	2640	CA	SER	Α	480	80.169	<b>7</b> 3.865	22.881	1.00	50.07
ATOM C	2641	С	SER	A	480	81.035	74.534	21.819	1.00	52.24
ATOM O	2642	0	SER	A	480	80.834	74.346	20.617	1.00	51.90
ATOM C	2643	CB	SER	A	480	79.085	74.842	23.351	1.00	50.84
ATOM O	2644	OG	SER	A	480	78.323	75.323	22.258	1.00	52.94
ATOM N	2645	N	VAL	A	481	82.015	75.301	22.288	1.00	54.50
ATOM C	2646	CA	VAL	A	481	82.929	76.029	21.416	1.00	56.91
ATOM C	2647	С	VAL	A	481	84.004	75.136	20.803	1.00	58.08
ATOM O	2648	0 .	VAL	A	481	84.966	75.637	20.216	1.00	58.99
ATOM C	2649	CB	VAL	A	481	83.641	77.154	22.193	1.00	57.54
ATOM C	2650	CG1	VAL	A	481	83.948	78.316	21.264	1.00	57.89
ATOM C	2651	CG2	VAL	Α	481	82.7,89	77.596	23.366	1.00	58.34
ATOM N	2652	N	SER	A	482	83.848	73.821	20.933	1.00	58.75
ATOM C	2653	CA	SER	A	482	84.838	72.896	20.393	1.00	59.46
ATOM C	2654	С	SER	A	482	84.252	71.737	19.593	1.00	60.06
ATOM O	2655	0	SER	A	482	83.245	71.896	18.902	1.00	60.14
ATOM C	2656	CB	SER	A	482	85.708	72.345	21.525	1.00	59.32

ATOM O	2657	OG	SER	A	482	86.717	71.486	21.025	1.00	60.01
ATOM N	2658	N	ILE	A	483	84.899	70.575	19.712	1.00	60.52
ATOM C	2659	CA	ILE	A	483	84.535	69.343	19.009	1.00	60.59
ATOM C	2660	С	ILE	A	483	85.319	69.317	17.701	1.00	60.24
ATOM O	2661	0	ILE	A	483	85.585	68.254	17.137	1.00	60.22
ATOM C	2662	CB	ILE	A	483	83.015	69.264	18.698	1.00	60.93
ATOM C	2663	CG1	ILE	A	483	82.227	69.079	19.997	1.00	60.99
ATOM C	2664	ÇG2	ILE	A	483	82.730	68.118	17.731	1.00	61.21
ATOM C	2665	CD1	ILE	A	483	80.725	69.039	19.804	1.00	60.52
ATOM N	2666	N	VAL	A	484	85.694	70.504	17.237	1.00	59.84
ATOM C	2667	CA	VAL	A	484	86.451	70.653	16.001	1.00	59.29
ATOM C	2668	С	VAL	A	484	87.845	70.049	16.151	1.00	58.69
ATOM O	2669	0	VAL	A	484	88.354	69.409	15.228	1.00	58.32
ATOM C	2670	СВ	VAL	A	484	86.590	72.145	15.612	1.00	59.56
ATOM C	2671	CG1	VAL	A	484	87.372	72.277	14.311	1.00	59.65
ATOM C	2672	CG2	VAL	A	484	85.209	72.775	15.469	1.00	59.42
ATOM N	2673	N	GLU	A	485	88.456	70.254	17.316	1.00	57.53
ATOM C	2674	CA	GLU	A	485	89.790	69.725	17.584	1.00	56.68
ATOM C	2675 ·	C	GLU	A	485	89.765	68.200	17.523	1.00	57.27
ATOM O	2676	0	GLU	A	485	90.758	67.565	17.164	1.00	56.78
ATOM C	2677	CB.	GLU	A	485	90.277	70.170	18.969	1.00	54.83
ATOM C	2678	CG	GLU	A	485	91.732	69.794	19.274	1.00	52.09
ATOM C	2679	CD	GLU	A	485	92.168	70.183	20.682	1.00	50.97
ATOM O	2680	OE1	GLU	A	485	91.768	69.499	21.649	1.00	45.34
ATOM O	2681	OE2	GLU	A	485	92.911	71.180	20.820	1.00	51.44
ATOM N	2682	N .	GLY	A	486	88.617	67.626	17.872	1.00	57.81
ATOM C	2683	CA	GLY	A	486	88.462	66.182	17.875	1.00	58.97
ATOM C	2684	C	GLY	A	486	88.580	65.524	16.515	1.00	59.51

ATOM O	2685	0	GLY.	A	486	89.142	64.435	16.398	1.00	59.72
ATOM N	2686	N	GLY	A	487	88.045	66.176	15.487	1.00	60.19
ATOM	2687	CA	GLY	A	487	88.118	65.620	14.146	1.00	60.96
C ATOM C	2688	С	GLY	A	487	89.336	66.120	13.394	1.00	61.44
ATOM O	2689	0	GLY	Α	487	90.170	66.831	13.957	1.00	61.56
ATOM N	2690	N	ALA	A	488	89.450	65.746	12.123	1.00	61.60
ATOM C	2691	CA	ALA	A	488	90.576	66.180	11.302	1.00	61.84
ATOM C	2692	С	ALA	A	488	90.446	67.683	11.068	1.00	62.10
MOTA	2693	0	ALA	A	488	89.365	68.171	10.739	1.00	61.91
O ATOM C	2694	CB	ALA	A	488	90.575	65.434	9.971	1.00	61.64
ATOM N	2695	N	HIS	Α	489	91.541	68.417	11.240	1.00	62.27
ATOM	2696	CA	HIS	Α	489	91.499	69.863	11.049	1.00	62.65
C ATOM C	2697	С	HIS	A	489	92.786	70.469	10.503	1.00	62.69
ATOM O	2698	0	HIS	A	489	93.887	70.008	10.809	1.00	62.31
ATOM	2699	CB	HIS	A	489	91.147	70.559	12.368	1.00	62.91
C ATOM C	2700	CG	HIS	A	489	92.100	70.258	13.484	1.00	63.07
ATOM N	2701	ND1	HIS	A	489	92.136	69.038	14.124	1.00	63.07
ATOM C	2702	CD2	HIS	A	489	93.060	71.016	14.066	1.00	63.14
ATOM C	2703	CE1	HIS	A	489	93.074	69.058	15.054	1.00	63.28
ATOM	2704	NE2	HIS	A	489	93.650	70.246	15.039	1.00	63.10
N ATOM N	2705	Ņ	ASP	A	490	92.626	71.513	9.695	1.00	62.96
ATOM C	2706	CA	ASP	A	490	93.747	72.234	9.101	1.00	62.99
ATOM C	2707	С	ASP	Α	490	94.619	71.381	8.187	1.00	63.25
ATOM	2708	0	ASP	A	490	95.824	71.609	8.066	1.00	62.96
O ATOM C	2709	СВ	ASP	A	490	94.593	72.857	10.210	1.00	63.04
ATOM C	2710	CG	ASP	A	490	93.789	73.797	11.086	1.00	63.29
ATOM	2711	OD1	ASP	A	490	93.394	74.879	10.597	1.00	62.95
O ATOM O	2712	OD2	ASP	A	490	93.539	73.447	12.259	1.00	63.21

ATOM N	2713	N	VAL	A	491	93.999	70.397	7.545	1.00	63.51
ATOM C	2714	CA	VAL	A	491	94.696	69.516	6.618	1.00	63.93
ATOM C	2715	С	VAL	A	491	93.743	69.145	5.489	1.00	64.46
ATOM O	2716	0	VAL	A	491	92.536	69.009	5.704	1.00	64.24
ATOM C	2717	СВ	VAL	A	491	95.188	68.214	7.308	1.00	63.80
ATOM C	2718	CG1	VAL	A	491	96.218	68.545	8.379	1.00	63.55
ATOM C	2719	CG2	VAL	A	491	94.010	67.464	7.913	1.00	63.70
ATOM N	2720	N	ILE	A	492	94.287	68.996	4.287	1.00	64.85
ATOM C	2721	CA	ILE	A	492	93.486	68.633	3.125	1.00	65.38
ATOM C	2722	С	ILE	A	492	93.564	67.121	2.911	1.00	65.68
ATOM O	2723	0	ILE	A	492	94.423	66.665	2.123	1.00	66.09
ATOM C	2724	CB	ILE	A	492	93.974	69.375	1.854	1.00	65.44
ATOM C	2725	CG1	ILE	A	492	93.922	70.887	2.084	1.00	65.23
ATOM C	2726	CG2	ILE	A	492	93.101	69.001	0.661	1.00	65.46
ATOM C	2727	CD1	ILE	A	492	94.390	71.707	0.900	1.00	65.68
TER	2728		ILE	A						
HETATM K		K	K		900	52.929	60.386	29.350	0.75	33.25
HETATM NA	2730	NA	NA		901	65.775	63.097	15.894	1.00	51.30
HETATM P	2731	P	RVP		602	67.806	55.192	15.010	1.00	32.06
HETATM O	2732	01P	RVP		602	67.447	55.106	13.566	1.00	33.43
HETATM O	2733	02P	RVP		602	68.618	53.993	15.386	1.00	33.48
HETATM O	2734	03 P	RVP		602	68.589	56.489	15.335	1.00	32.27
HETATM O	2735	05*	RVP		602	66.564	55.260	15.998	1.00	32.66
HETATM C	2736	C5*	RVP		602	65.601	54.207	15.962	1.00	31.36
HETATM C	2737	C4*	RVP		602	64.521	54.418	16.985	1.00	30.66
HETATM O	2738	04*	RVP		602	63.766	55.605	16.540	1.00	29.94
HETATM C	2739	C3*	RVP		602	63.437	53.370	17.179	1.00	29.26
HETATM O	2740	03*	RVP		602	63.863	52.229	17.914	1.00	28.74
HETATM C	2741	C2*	RVP		602	62.343	54.162	17.832	1.00	30.26

HETATM O	2742	02*	RVP	602	62.482	54.278	19.236	1.00	30.38
HETATM C	2743	C1*	RVP	602	62.434	55.486	17.067	1.00	31.26
HETATM N	2744	N9	RVP	602	61.475	55.602	15.903	1.00	32.47
HETATM C	2745	C8	RVP	602	60.989	54.694	14.978	1.00	33.70
HETATM N	2746	N7	RVP	602	60.171	55.231	14.129	1.00	33.53
HETATM C	2747	C5	RVP	602	60.084	56.544	14.468	1.00	34.69
HETATM C	2748	C6	RVP	602	59.329	57.634	13.877	1.00	34.93
HETATM O	2749	06	RVP	602	58.592	57.567	12.906	1.00	35.34
HETATM N	2750	N1	RVP	602	59.501	58.902	14.532	1.00	35.14
HETATM N	2751	N4	RVP	602	60.883	56.810	15.574	1.00	33.87
HETATM O	2752	0	нон	1	75.701	41.635	35.059	1.00	43.94
HETATM O	2753	0	НОН	2	74.079	38.696	40.465	1.00	55.18
HETATM O	2754	0	нон	3 .	65.938	60.588	24.743	1.00	24.75
HETATM O	2755	0	нон	4	90.376	44.734	34.332	1.00	58.18
HETATM O	2756	0	НОН	5	57.606	58.768	28.316	1.00	26.20
HETATM O	2757	0	нон	6	73.742	57.520	36.339	1.00	22.08
HETATM O	2758	0	нон	7	59.439	45.332	37.045	1.00	28.29
HETATM O	2759	0	нон	8	66.630	48.045	39.016	1.00	24.24
HETATM O	2760	0	нон	9	87.313	55.537	31,236	1.00	26.94
HETATM O	2761	0	НОН	10	79.723	41.990	29.591	1.00	24.41
HETATM O	2762	0	НОН	11	70.855	54.607	21.999	1.00	25.98
HETATM O	2763	0	нон	12	75.110	45.838	32.838	1.00	30.43
HETATM O	2764	0	нон	13	71.016	53.391	14.308	1.00	28.65
HETATM O	2765	0	нон	14	75.872	56.829	34.478	1.00	29.47
HETATM O	2766	0	нон	15	84.437	53.172	21.050	1.00	27.86
HETATM O	2767	0	нон	16	76.208	43.857	31.117	1.00	21.58
HETATM O	2768	0	нон	17	88.575	53.835	33.310	1.00	28.69
HETATM O	2769	0 .	НОН	18	78.805	48.189	37.292	1.00	30.37

нетатм	2770	0	нон	19	81.282	64.691	32.797	1.00	26.40
O HETATM	2771	0	нон	20	74.258	59.955	37.886	1.00	35.26
0							,		
HETATM O	2772	0	нон	21	72.681	38.221	33.950	1.00	27.93
HETATM O	2773	0	нон	22	56.779	57.580	38.836	1.00	33.24
HETATM O	2774	0	нон	23	69.275	68.052	32.909	1.00	34.10
HETATM	2775	0	нон	24	58.760	51.196	23.042	1.00	28.36
O HETATM O	2776	0	нон	25	79.310	40.417	32.071	1.00	30.06
HETATM O	277 <b>7</b>	0	нон	26	77.754	54.034	34.410	1.00	31.27
HETATM O	2778	0	НОН	27	64.140	56.432	20.380	1.00	35.64
HETATM O	2779	0	нон	28	62.442	38.699	34.139	1.00	30.68
нетатм	2780	0	нон	29	65.481	36.753	34.839	1.00	29.52
OHETATM	2781	0	нон	30	49.387	44.266	21.091	1.00	32.82
OHETATM	2782	0	нон	31	74.171	50.758	36.345	1.00	35.61
O HETATM O	2783	0	нон	32	76.573	41.279	32.222	1.00	30.60
HETATM O	2784	0	нон	33	87.348	67.083	31.015	1.00	29.38
HETATM O	2785	0	НОН	34	66.425	37.664	16.827	1.00	27.26
HETATM O	2786	0	нон	35	59.765	51.154	9.792	1.00	31.75
HETATM O	2787	0	нон	36	61.770	50.532	17.896	1.00	26.41
HETATM O	2788	0	нон	37	65.804	58.780	21.469	1.00	36.21
HETATM O	2789	0	нон .	38	76.213	52.726	36.406	1.00	34.08
HETATM O	2790	0	нон	39	59.631	51.746	16.407	1.00	31.30
HETATM O	2791	0	НОН	40	82.391	67.258	31.863	1.00	31.37
HETATM O	2792	0	нон	41,	70.252	33.623	27.556	1.00	35.71
HETATM O	2793	0	НОН	42	72.039	67.304	32.099	1.00	35.67
HETATM O	2794	0	нон	43	53.140	51.705	38.165	1.00	31.55
HETATM O	2795	0	нон	44	67.908	38.414	46.440	1.00	32.54
HETATM O	2796	0	нон	45	58.797	45.284	6.070	1.00	39.86
HETATM O	2797	0	нон	46	50.916	46.272	35.836	1.00	39.05

НЕТАТМ О	2798	0	нон	47	48.468	54.286	36.992	1.00	37.90
HETATM O	2799	0	НОН	48	79.368	38.350	17.558	1.00	37.55
HETATM O	2800	0	нон	49	65.917	31.312	26.738	1.00	40.60
HETATM O	2801	0	нон	50 、	75.195	38.963	31.142	1.00	31.97
HETATM O	2802	0	нон	51	51.201	58.619	25.886	1.00	40.51
HETATM O	2803	0	НОН	52	56.361	77.266	37.184	1.00	34.64
HETATM O	2804	0	нон	53	75.373	38.767	8.255	1.00	34.82
HETATM O	2805	0	нон	54	62.203	64.463	35.439	1.00	32.93
HETATM O	2806	0	НОН	55	67.513	69.374	38.251	1.00	43.30
HETATM O	2807	0	НОН	56	59.023	38.343	34.814	1.00	35.89
HETATM O	2808	0	нон	57	61.282	73.583	39.232	1.00	39.52
HETATM O	2809	0	нон	58	74.916	47.914	35.808	1.00	36.57
HETATM O	2810	0	нон	59	62.673	61.732	37.514	1.00	33.12
HETATM O	2811	0	нон	60	74.787	37.123	10.828	1.00	36.31
HETATM O	2812	0	нон	61	87.050	70.287	23.795	1.00	40.37
HETATM	2813	0	нон	62	60.963	37.766	37.311	1.00	46.47
HETATM O	2814	0	нон	63	74.898	62.998	19.440	1.00	40.44
HETATM O	2815	0	НОН	64	60.204	41.357	39.977	1.00	48.22
HETATM O	2816	0	НОН	65	83.322	55.796	16.450	1.00	32.01
HETATM O	2817	0	нон	66	74.375	34.757	40.315	1.00	36.09
HETATM O	2818	0	нон	67	71.494	55.957	41.977	1.00	32.49
HETATM O	2819	0	нон	68	59.957	50.992	20.176	1.00	43.21
HETATM O	2820	0	нон	69	66.080	28.763	15.101	1.00	39.12
HETATM O	2821	0	нон	70	50.588	31.847	16.621	1.00	43.31
HETATM O	2822	0	нон	71	69.529	68.913	36.005	1.00	40.30
HETATM O	2823	0	нон	72	73.768	64.532	30.646	1.00	40.71
HETATM O	2824	0	нон	73	92.829	49.112	23.281	1.00	44.30
HETATM O	2825	0	нон	74	70.278	54.233	17.770	1.00	32.36

TABLE 7 . 485

HETATM O	2826	0	нон	75	52.179	53.975	25.940	1.00 38.86
HETATM O	2827	0 -	нон	76	70.150	32.823	38.265	1.00 49.16
HETATM O	2828	0	НОН	77	69.559	45.202	46.424	1.00 37.45
HETATM O	2829	0	нон	78	81.658	38.524	24.274	1.00 39.74
HETATM O	2830	0	нон	79	85.501	49.287	39.572	1.00 41.67
HETATM O	2831	0	НОН	80	43.313	43.736	23.528	1.00 38.76
HETATM O	2832	0	нон	81	45.058	35.260	19.329	1.00 48.10
HETATM O	2833	0	нон	82	86.888	47.694	13.726	1.00 42.11
HETATM O	2834	0	НОН	83	59.990	59.432	31.077	1.00 43.45
HETATM O	2835	0	нон	84	65.702	28.237	26.872	1.00 41.07
HETATM O	2836	0	нон	85	56.392	41.602	37.511	1.00 42.34
HETATM O	2837	0	НОН	86	89.958	53.438	35.939	1.00 44.28
HETATM O	2838	0	нон	87	53.813	58.314	38.115	1.00 43.91
HETATM O	2839	0	НОН	88	54.846	33.441	37.762	1.00 45.87
HETATM O	2840	0	НОН	89	68.555	74.630	33.270	1.00 45.09
HETATM O	2841	0	нон	90	46.075	48.997	27.411	1.00 39.29
HETATM O	2842	0	нон	91	58.611	35.738	27.091	1.00 37.48
HETATM O	.2843	0	нон	92	65.536	61.610	38.426	1.00 47.43
HETATM O	2844	0	нон	93	63.014	78.411	34.747	1.00 48.43
HETATM O	2845	0	нон	94	69.402	35.849	7.804	1.00 43.16
HETATM O	2846	0:	НОН	95 🖰	51.178	50.724	21.941	1.00 39.55
HETATM O	2847	0	НОН	96	85.871	39.272	22.557	1.00 42.34
HETATM O	2848	0	нон	97	55.141	46.898	17.592	1.00 50.68
HETATM O	2849	0	нон	98	54.804	53.900	40.431	1.00 53.97
HETATM O	2850	0	НОН	99	81.143	54.940	13.409	1.00 49.06
HETATM O	2851	0	нон	100	60.601	30.026	22.828	1.00 51.45
HETATM O	2852	0	нон	101	91.377	38.681	33.317	1.00 51.98
HETATM O	2853	0	нон	102	50.491	32.970	12.092	1.00 45.61

HETATM O	2854	0	нон	103	65.951	63.935	21.639	1.00 45.	03
HETATM O	2855	0	нон	104	92.613	40.981	20.428	1.00 51.	23
HETATM O	2856	0	НОН	105	66.842	34.584	37.015	1.00 49.	51
HETATM O	2857	0	нон	106	79.154	37.014	24.773	1.00 43.	76
HETATM O	2858	0	нон	107	72.247	31.318	24.007	1.00 40.	85
HETATM O	2859	0	нон	108	60.754	51.022	46.130	1.00 52.	32
HETATM O	2860	0	нон	109	45.352	44.922	33.115	1.00 39.	72
HETATM O	2861	0	нон	110	43.049	56.846	35.553	1.00 56.	39
HETATM O	2862	0	НОН	111	93.844	47.843	37.235	1.00 47.	50
HETATM O	2863	0	нон	112	72.886	49.728	42.684	1.00 42.	85
HETATM O	2864	0	нон	113	44.622	43.340	15.564	1.00 48.	15
HETATM O	2865	0	нон	114	56.638	31.718	23.687	1.00 50.	30
HETATM O	2866	0	нон	115	75.960	53.691	-1.202	1.00 54.	62
HETATM O	2867	0	нон	116	63.275	58.904	18.617	1.00 44.	23
HETATM O	2868	0	нон	117	58.451	52.848	43.791	1.00 49.	56
HETATM O	2869	0	нон	118	54.165	41.889	6.948	1.00 52.	21
HETATM O	2870	0	нон	119	49.652	53.672	24.234	1.00 60.	78
HETATM O	2871	0	НОН	120	53.791	55.765	20.073	1.00 41.	34
HETATM O	2872	0	нон	121	82.081	63.415	21.222	1.00 39.	55
HETATM	2873	0	нон	122	59.793	54.194	20.862	1.00 39.	76
HETATM O	2874	O .	нон	123	91.395	41.899	35.234	1.00 47.	28
HETATM O	2875	Ο.	нон	124	78.660	72.133	28.009	1.00 48.	50
HETATM O	2876	0	нон	125	76.816	36.477	6.733	1.00 59.	31
HETATM O	2877	0	нон	126	51.697	56.879	39.951	1.00 56.	83
HETATM O	2878	0	нон	127	73.160	41.047	42.151	1.00 46.	35
HETATM O	2879	0	нон	128	78.361	33.624	16.246	1.00 47.	03
HETATM O	2880	0	нон	129	65.071	63.965	35.876	1.00 40.	53
HETATM O	2881	0	нон	130	75.546	70.802	31.702	1.00 43.	13

HETATM O	2882	0	нон	131	45.695	41.554	13.117	1.00	46.21
HETATM O	2883	0	нон	132	74.770	75.486	30.649	1.00	50.17
HETATM	2884	0	нон	133	61.457	33.492	27.149	1.00	38.92
O HETATM O	2885	0	нон	134	78.747	70.267	25.631	1.00	47.28
HETATM O	2886	0	нон	135	67.587	59.325	38.812	1.00	44.68
HETATM O	2887	0	нон	136	56.460	34.436	25.338	1.00	50.36
HETATM O	2888	0	нон	137	87.425	55.130	37.159	1.00	57.77
HETATM O	2889	0	нон	138	62.549	55.054	1.389	1.00	52.64
HETATM O	2890	0	НОН	139	63.046	39.459	6.185	1.00	33.80
HETATM O	2891	0	нон	140	52.457	45.986	7.697	1.00	51.12
HETATM O	2892	0	нон	141	68.162	53.372	47.262	1.00	59.06
HETATM	2893	0	нон	142	54.370	73.869	39.160	1.00	53.30
OHETATM	2894	0	нон	143	58.332	49.599	44.654	1.00	56.73
O HETATM	2895	0	нон	144 .	57.914	66.131	38.178	1.00	50.57
O HETATM O	2896	0	нон	145	69.153	44.094	0.472	1.00	58.32
HETATM	2897	0	нон	146	70.955	57.555	14.580	1.00	42.14
O HETATM O	2898	0	нон	147	64.290	80.942	33.633	1.00	50.16
HETATM O	2899	0	нон	148	71.059	63.093	33.999	1.00	48.63
HETATM O	2900	0	нон	149	68.250	44.131	48.927	1.00	56.50
HETATM O	2901	0	нон	150	53.995	61.899	36.136	1.00	38.46
HETATM O	2902	0	нон	151	61.723	64.570	38.471	1.00	57.73
HETATM O	2903	0	нон	152	72.479	45.867	47.190	1.00	59.67
HETATM O	2904	0	нон	153	72.416	63.521	16.449	1.00	43.93
HETATM O	2905	0	нон	154	72.663	61.263	18.483	1.00	55.81
HETATM O	2906	0	нон	155	78.290	65.312	33.155	1.00	53.08
HETATM O	2907	0	нон	156	94.608	53.219	22.065	1.00	52.11
HETATM	2908	0	нон	157	75.671	73.066	28.735	1.00	53.82
HETATM O	2909	0	нон .	158	75.598	67.940	32.952	1.00	59.45

HETATM	2910	0	нон	159	75.773	35.559	27.231	1.00	45.26
O HETATM	2911	0	нон	160	97.730	48.875	26.955	1.00	50.24
OHETATM	2912	0	нон	161	95.855	46.417	27.517	1.00	51.32
O HETATM O	2913	0	нон	162	94.096	48.923	26.023	1.00	51.83
HETATM O	2914	0	нон	163	91.721	50.895	35.397	1.00	58.59
HETATM O	2915	0	нон	164	92.397	47.915	34.455	1.00	52.43
HETATM O	2916	0	нон	165	97.410	43.546	26.476	1.00	59.63
HETATM O	2917	0	нон	166	90.165	38.748	36.119	1.00	56.38
HETATM O	2918	0	-HOH	167	94.316	37.414	34.403	1.00	54.53
HETATM	2919	0	нон	168	43.075	36.122	24.970	1.00	55.92
OHETATM	2920	0	нон	169	67.736	76.231	16.895	1.00	56.81
O HETATM	2921	0	НОН	170	71.677	32.859	30.158	1.00	52.78
OHETATM	2922	0	нон	171	68.554	30.002	38.857	1.00	54.82
O HETATM	2923	0	нон	172	73.000	33.391	26.251	1.00	47.75
O HETATM	2924	0	нон	173	68.812	31.473	26.121	1.00	56.59
OHETATM	2925	0	нон	174	63.228	31.574	25.697	1.00	48.31
O HETATM O	2926	0	нон	175	62.682	33.531	30.030	1.00	49.27
HETATM O	2927	0	нон	176	65.167	31.555	29.683	1.00	55.99
НЕТАТМ	2928	0	нон	177	56.336	48.164	14.845	1.00	48.86
O HETATM	2929	, <b>O</b>	нон	178	78.620	50.501	10.475	1.00	62.38
OHETATM	2930	0	нон	179	84.701	43.066	9.965	1.00	56.01
O HETATM	2931	0	нон	180	77.072	52.215	-3.925	1.00	52.09
O HETATM	2932	0	нон	181	81.505	72.460	16.927	1.00	56.81
O HETATM O	2933	0	нон	182	56.776	62.766	36.110	1.00	35.88
HETATM	2934	0	нон	183	52.708	50.106	19.084	1.00	46.95
O HETATM	2935	0	нон	184	58.949	41.892	6.150	1.00	50.09
O HETATM O	2936	0	нон	185	66.279	40.996	3.132	1.00	51.65
HETATM O	2937	0	нон	186	72.364	36.495	6.684	1.00	54.90

HETATM O	2938	0	нон	187		64.663	41.304	7.894	1.00 34.55
HETATM O	2939	0	нон	188		49.873	42.836	7.978	1.00 55.76
HETATM O	2940	0	нон	189	•	57.589	27.901	17.205	1.00 55.94
HETATM O	2941	0	нон	190		54.487	27.148	17.217	1.00 56.50
HETATM O	2942	0	нон	191		74.055	29.387	14.028	1.00 55.18
HETATM O	2943	0	НОН	192		73.877	34.935	8.889	1.00 54.31
HETATM O	2944	0	нон	193		64.874	25.940	14.827	1.00 47.78
HETATM O	2945	0	нон	194		40.739	38.113	26.191	1.00 56.93
HETATM O	2946	0	нон	195		81.037	48.857	11.250	1.00 51.13
HETATM O	2947	0	НОН	196		43.149	34.719	28.062	1.00 59.10
HETATM O	2948	0	нон	197		63.348	58.590	43.529	1.00 57.64
HETATM O	2949	0	нон	198		48.595	31.656	25.612	1.00 58.04
HETATM O	2950	0	НОН	199		58.778	58.864	41.117	1.00 54.64
HETATM O	2951	0	нон	200		52.055	49.602	40.062	1.00 50.74
HETATM O	2952	0	нон	201		55.370	44.532	39.918	1.00 58.59
CONECT	202	2494							
CONECT									
CONECT			1503	1505					
CONECT				1303					
CONECT									
CONECT								•	
CONECT			1500						
CONECT									
CONECT		202							
CONECT			2733	2734	2735				
CONECT			2,33	2,51	2,33		0		
CONECT									
CONECT			•						
CONECT			2736	•					
CONECT									
CONECT				2739					
CONECT				2,33					
CONECT				2741					
CONECT			/ ·± U	<del></del> .					
CONECT			2742	2742					
CONECT			4174	2143					
CONECT			27/1	27/1			•		
CONECT									
CONECT				4/3I					
CONECT									
				2753					
CONECT									

CONECT 2749 2748 CONECT 2750 2748

CONECT 2751 2744 2747

MASTER 497 0 4 14 18 0 0 6 2951 1 30 39

END

TABLE 8. Comparison of published IMPDH structures.

Species	Resolution	R (R _{free} ) in %	Missing residues	Heteroatoms	PDB ID
Human	2.9 Å	24.4 (27.0)	2 nd domain 130-139, 159-177,	CPR, SAD	1B30
		,	flap 400-448, end 499-514		
Hamster	2.6 Å	21.7 (28.5)	2 nd domain 121-177, flap 421-	K⁺, XMP*,	1JR1
			436	MPA	
Borrelia	2.4 Å	21.5 (26.8)	2 nd domain 92-129, flap 309-	SO ₄ ⁺	1EEP
			344		
S. pyogenes	1.9 Å	23.4 (25.8)	Flap 401-414, end 490-493	IMP	1ZFJ
T. foetus apo	2.3 Å	21.8 (26.5)	2 nd domain 102-221, loop	SO ₄ ⁺	1AK5
			314-327, flap 413-431		
T. foetus +	2.6 Å	20.3 (26.4)	2 nd domain 102-221, loop	XMP	. N/A
XMP		,	314-324, flap 413-431, end		
			484-503		

^{*} denotes covalent intermediate

**TABLE 9** Data collection and refinement statistics.

Structure	RMP	RMP+MPA
Wavelength (Å)	0.97	0.97
Resolution range (Å)	50-1.90	50-2.15
Resolution of outer shell (Å)	1.90-2.02	2,15-2.28
Current R (R _{FREE} ) (%)	24.3 (25.9)	23.3 (26.5)
Unique reflections	50,359	35,250
Total observations	1,289,813	620,781
I/σ _I overall/outer shell	33.77/2.39	23.59/2.05
R _{sym} overall/outer shell (%)	6.2/68.9	7.2/49.1
Completeness overall/outer shell (%)	99.9/100	94.0/79.5
Degrees collected	25	20
Number of ordered water molecules	211	120
Deviation from ideal bond lengths (Å)	0.005	0.006
Bond angle RMSD (°)	1.2	1.2
Dihedral angle RMSD (°)	22.7	22.6
Improper angle RMSD (°)	0.71	0.70
Cell dimensions $\alpha=\beta=\chi=90^{\circ}$ , $a=b=c$ (Å)	154.7	155.1
Space group	P432	P432
Mosaicity (°)	0.45	0.50